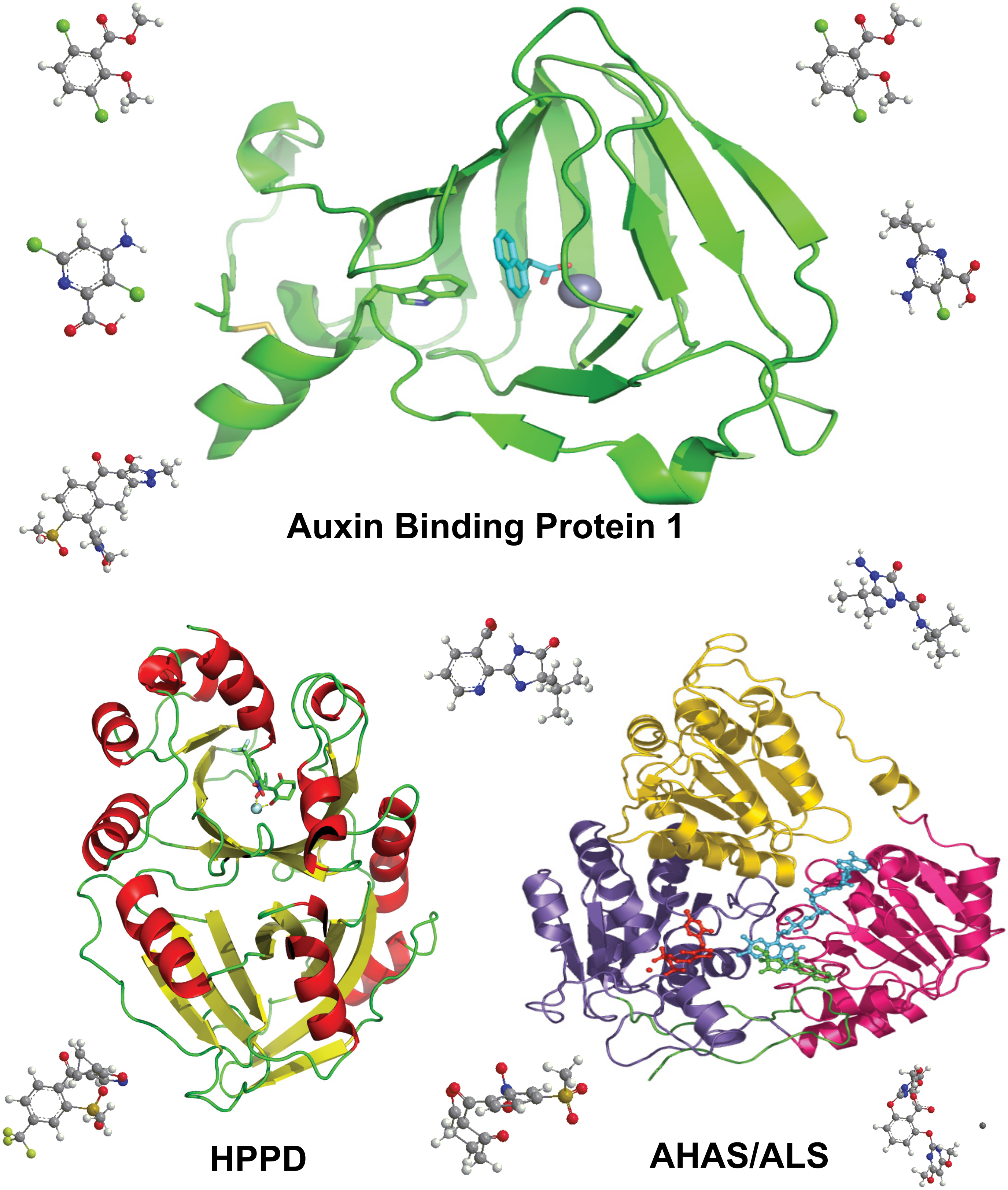
Herbicide Handbook

Weed Science Society of America

Tenth Edition, 2014



HERBICIDE HANDBOOK

TENTH EDITION
2014
Editor: Dale L. Shaner
Herbicide Handbook Committee

D.L. Shaner (chair)
Shaner Consulting
Fort Collins, CO

J. J. .Jachetta
DowAgro Science
Indianapolis, IN

S. Senseman
University of Tennessee
Knoxville, TN

I. Burke
Washington State University
Pullman, WA

B. Hanson
University of California
Davis, CA

M. Jugulam
Kansas State University
Manhattan KS

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Ralegih, NC

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Syngenta Crop Protection
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Bayer Crop Science
Frankfort, Germany

R. McAllister
Crop Life America
Washington, DC

J. Green
Pioneer
Ames, IA

B. Glenn
Crop Life America
Washington, DC

P. Turner
Gowan
Yuma, AZ

J. Pawlak
Valent
Lansing, MI.

Published by

Weed Science Society of America
810 E. 10th Street
Lawrence, KS 66044-8897
U.S.A.

ISBN 978-0-615-98937-2

The *Herbicide Handbook* of the Weed Science Society of America was first published in 1967. It was, and continues to be, the work of WSSA's Herbicide Handbook Committee. Each edition is dedicated to an individual recognized for outstanding service and accomplishments in herbicide technology. Publication dates and dedication recipients are listed below.

Edition	**Year**	**Dedicated to**
First published	1967	Marion W. Parker
Second edition	1970	Kenneth P. Buchholtz
Third edition	1974	Charles J. Willard
Fourth edition	1979	Alden S. Crafts
Fifth edition	1983	Robert H. Beatty
Sixth edition	1989	F. Leonard Timmons
Seventh edition	1994	Fred W. Slife
Eight edition	2002	Dan Hess & Fred Warren
Ninth edition	2007	Kriton K. Hatzios
Tenth Edition	2014	John Wilcut & Homer LeBaron

Chemicals presented in previous editions of the *Herbicide Handbook* that are currently of minimal interest or have not been produced for several years have been omitted from this edition. Such chemicals are listed on page 414. Earlier editions should be retained to maintain a record of past and present herbicides.

Cover design by Dale L. Shaner
Auxin Binding Protein 1: Crystal structure of naphthalene acetic acid (stick representation in cyan) bound to the metal ion (gray sphere) at the active centre of ABP1 (PDB accession code:1LRH; Woo et. al. (2002) EMBO J. 21, 2877-2885). With permission from Dr Richard W Pickersgill

HPPD (4-hydroxyhenyl-pyruvatedioxygenase): Crystal structure of NTBC bound to active site of HPPD. Adapted from J. Brownlee, K. Johnson-Winters, D. H. T. Harrison and G. R. Moran (2004) Biochemistry 43, 6370-6377 by G.R. Moran.. With permision from Dr. Graham R. Moran

AHAS/ALS (acetohydroxyacid synthase/acetolactate synthase). Stucture with sulfometuron methyl in its binding site adapted by Jennifer McCourt from Fig. 1B of McCourt, J.A., Pang, S.S., King-Scott, J., Guddat, L.W., Duggleby, R.G.: (2006) Proc. Natl.Acad.Sci.Usa 103: 569-573. With permission from Dr. R..G. Duggleby

Contents

Homer McKay LeBaron

iWhen Dr. Homer LeBaron passed away in June of 2012, he left behind an important legacy as a researcher, mentor, educator, agricultural leader and promoter of the weed science profession.

Born in 1926 in Alberta, Canada, Dr. LeBaron earned B.S and M.S. degrees at Utah State University, and a Ph.D. at Cornell University. He was supported in all his endeavors by his first wife Venita Vance for 38 years until her passing in 1990, and by his second wife Aleene Sumsion for 21 years. Their loving family includes seven children, five step-children, and a growing posterity.

Dr. LeBaron worked with Geigy Chemical Corporation (now Syngenta), where he rose through the ranks to became a senior research fellow in biochemistry, new technology and basic research. During that period he became one of the world's leading authorities on weed science and herbicide modes of action including the triazine herbicides and their role in revolutionizing weed control to benefit food production.

He also became a respected spokesperson on many of the most important issues in agriculture, and research and development.   He was one of the first scientists to understand the global significance of the emerging problem of herbicide resistance. He spearheaded symposia, wrote and delivered many papers on the topic, and helped to launch a new generation of science-based best practices in integrated weed management.

The USDA awarded Dr. LeBaron a Certificate of Appreciation for outstanding leadership in groundwater research programs. In addition, he was the first scientist from industry to receive the Council for Agricultural Science and Technology's Charles A. Black Award – a recognition acknowledging his outstanding achievements in promoting sound science and a public understanding of agriculture.

Dr. LeBaron also was an active proponent of the weed science profession. He became the first individual to lead three separate weed science societies, serving as president of the Weed Science Society of America, the Northeastern Weed Science Society and the Southern Weed Science Society.

He was an active member of the International Weed Science Society, American Society of Agronomy, American Chemical Society, Entomological Society of America, American Phytopathological Society, Council for Agricultural Science and Technology, Sigma Xi Scientific Research Society, Aquatic Plant Management Society and European Weed Research Society.

He also was the author or coauthor of 90 publications, including six books and multiple special reports.

Dr. LeBaron was not only a respected scientist, but also a kind and gentle man who lived a life of service to church and community, including missions in France and Africa. He is held in high esteem by his family, many friends and colleagues around the globe. He is greatly missed.

John Wilcut

Dr. John William Wilcut passed to his final rest on August 24, 2007, following a valiant struggle with cancer. He was born in Farmington, MO in 1955 and grew up in a small town in central Illinois. He received his B.S. and M.S. degrees in botany from Eastern Illinois University at Charleston. He completed his Ph.D. in weed science and plant physiology at Auburn University in 1986 and worked the following year as a post-doctoral research associate at Auburn.

John joined the faculty of VPI&SU in 1987 as extension weed science specialist at the Tidewater Agricultural Research and Extension Center in Suffolk. At Suffolk, John worked tirelessly to develop a well-respected extension program supported by his extensive applied research. In 1990, he accepted a research position with the University of Georgia at the Coastal Plain Experiment Station in Tifton where he conducted a very extensive research program on cotton and peanut weed management. John's desire to be on a main campus and to teach and interact with students led him to the Crop Science Department at North Carolina State University in 1994. He was promoted to professor in 2000.

Dr. Wilcut was recognized nationally and internationally for his extensive work and leadership in the areas of weed management, weed biology, and herbicide physiology. He was well known for the productivity of his program, his collaborative research with colleagues around the country, and his keen insight and ability to find solutions to weed management problems facing producers. His expertise led to numerous invitations to speak at field days and commodity and industry meetings and to advise regulatory groups. He received well over four million dollars in program support over his career. John's efforts and collaboration with graduate students and other professional colleagues resulted in over 200 journal publications, five book chapters, and hundreds of abstracts.

Dr. Wilcut's greatest professional passion was mentoring students. He attracted some of the best graduate students in the country, and 20 students completed advanced degrees under his guidance. John's program was rigorous and demanding, and by example he set high expectations. John insured his students were well trained, and he instilled into his students a strong work ethic and a desire to excel. His students received recognition through numerous awards from the Weed Science Society of America, the Southern Weed Science Society, the American Peanut Research and Education Society, the National Cotton Council, and other professional groups. All of his students are now into successful careers in academia and private industry and readily acknowledge the impact John had on their professional development. John also taught the undergraduate weed science course at N. C. State with equal passion for the subject and high expectations from students. His dedication to the educational and professional development of undergraduates was recognized with receipt of the Outstanding Faculty Member Award from the Agronomy Club.

Dr. Wilcut was a member of the Weed Science Society of America, the Southern Weed Science Society, the American Peanut Research and Education Society, and the Beltwide Cotton Weed Science Research Conference. He served on numerous committees and organized symposia and he was always an active participant in meetings of those groups. He served as Editor of Weed Technology from 2003 until his death in 2007. He also served as Editor of Peanut Science from 2005 until 2007. Many members of the American Peanut Research and Education

Society credit John with revitalizing their flagship publication Peanut Science.

John received numerous awards recognizing his excellence in research and education, including Outstanding Young Weed Scientist, Outstanding Educator, and Weed Scientist of the Year from the Southern Weed Science Society; induction as Fellow and recipient of the Early Career Award and Outstanding Teacher Award from the Weed Science Society of America; and the Dow AgroSciences Research Award and the Bailey Award from the American Peanut Research and Education Society.

Dr. Wilcut will be remembered by his professional family for his passion for weed science, his impact on the profession, and his competitive nature. John was a fighter, a trait that served him well during his illness. He will also be remembered for his candid opinions and his willingness to mentor junior colleagues and help them with their professional development.

Dr. Wilcut approached his personal life with the same zeal and dedication to family that we remember from his professional life. He was a loving and supportive husband and caring father exceedingly proud of his children and their accomplishments. In spite of long hours devoted to career, John made and cherished personal time with family. He particularly enjoyed sporting events and family beach vacations. John is survived by his wife Cathy, his son Jared, and his daughter Caitlyn.

PREFACE

The tenth edition of the *Herbicide Handbook* includes information on more than 200 herbicides and a few other chemicals such as safeners, modifiers, and extenders for herbicides, desiccants, and plant growth regulators. We have made several substantial changes to the format of the book in this edition to hopefully make it more user-friendly and to remove some redundancies. The listing of the herbicides is now in alphabetical order and each herbicide has its own section. The pages have been designed to show the common names, the CAS chemical name, and the CAS reference number and the Weed Science Society of America (WSSA) and the Herbicide Resistance Action Committee's designation code for primary sites of action at the top of each entry.

The manufacturer's information is at the end of each entry wherease the trade names are listed at the front of each entry. As in the last edition the way that the chemicals are presented the same information categories for each compound. Details about the mechanism of action is referenced to the Mechanism of Action section at the beginning of the book.

The Mechanism of Action Classification has been updated to the latest version with several new categories as sanctioned by WSSA and HRAC and goes into more detail about each site of action rather than repeating this detail within each entry.

Information for this handbook has been collected through contacts with individuals working for the manufacturers (sometimes more than one), material safety data sheets (MSDS), chemical labels, scientific articles, original data, government databases, and earlier versions of the *Herbicide Handbook*.

A number of values for water solubility, K_{oc}, field dissipation half-life in soil, and pK_a were taken from the SCS/ARS/CES Pesticide Properties Database (see Rev. Environ. Contam. Toxicol., Vol. 123 (1992) and Vol. 137 (1994)) and are referenced accordingly. Values for K_{oc} and half-life in soil from this data base must be considered "average" or "typical" and to be used with discretion as an approximate characterization of the chemical when more specific values are lacking. Caution is advisable in use of such numbers because K_{oc} and soil half-life may be affected significantly by several soil properties and environmental factors.

A standardized system of descriptions and two-letter abbreviations for formulation types was adopted for use in the eighth edition of the *Herbicide Handbook*. The system has been prepared by the International Group of National Associations of Agrochemical Manufacturers (GIFAP) and is detailed in a document entitled GIFAP Catalogue of Pesticide Formulation Types and International coding System (Jan. 1984, Brussels). The GIFAP formulation descriptions are given in the Abbreviations and Symbols section in the back of the book.

We sought information on all current herbicides (active ingredients and formulated products), regardless of availability in the United States. Any current active ingredient not found as an entry in this handbook indicates a lack of sufficient information made available to the committee. Failure of the handbook to list certain product trademarks by company under the appropriate active ingredient entry does not imply endorsement of one product over another. Companies wishing to submit product information for the next handbook edition should contact WSSA.

The *Herbicide Handbook* is designed principally for use by research, teaching, and extension personnel at academic institutions as well as by industry or government representatives. Information on herbicide use in the *Herbicide Handbook* are not meant to serve as recommendations or to take the place of recommendations published by the manufacturer. Use recommendations should be obtained only from the product labels.

Companies whose products are mentioned in this edition have been listed to show their contact information. The index in the back of the book contains common names (lower case), code names, trade names (upper case), and chemical family names for handbook entries. Chemicals included in previous editions but omitted from earlier editions have not been indexed.

Data included herein are based on extensive research, and care has been taken to ensure accuracy insofar as possible. However, the suppliers of this information and the *Herbicide Handbook* Committee make no warranty of any kind as to its accuracy or utility. The committee encourages notification of omissions and errors to assist in improving subsequent editions.

Publication of the *Herbicide Handbook* was made possible by the cooperation of industry representatives and *Herbicide Handbook* committee members who spent considerable time and effort obtaining data for new chemical entries. The *Herbicide Handbook* chair sincerely appreciates these efforts.

The chair would also like to thank Mr. Alan Wood for his help and use of his website www.alanwood.net/pesticides and his Compendium of Pesticide Common Names. Cross-referencing structures and chemical names would have been much more difficult without this useful resource. Other web-based cites that were very useful in cross-referencing information in the handbook were the following:

http://www.cdms.net/
http://www.epa.gov
http://www.greenbook.net/
http://www.pesticideinfo.org/
http://www.weedscience.org/summary/

Thanks also to the past chair, Dr. Scott Sensemen, for his advice and help on the committee. Thanks to Dr. Sarah Ward for her help and support as the Director of Publications for WSSA during the development of this handbook. Thanks to Allen Press for their help and guidance.

Thanks to Dr. Allen Appleby for the use of his Herbicide Geneology.

Thanks to Dr. Alan York and Dr. Janis McFarland for their help in the dedication material for Dr. John Wilcutt and Dr. Homer LeBaron, respectively.

Finally, I would like to thank my wife, Diana, for her love and support during this ambitious undertaking.

Dale Shaner, Editor
May, 2014

Summary of Herbicide Mechanism of Action According to the Weed Science Society of America (WSSA) and the Herbicide Resistance Action Committee (HRAC) Classification

1$^{(A)}$ Acetyl CoA Carboxylase (ACCase) Inhibitors

Aryloxyphenoxypropionate (FOPs) and cyclohexanedione (DIMs) herbicides inhibit the enzyme acetyl-CoA carboxylase (ACCase), the enzyme catalyzing the first committed step in *de novo* fatty acid synthesis (Burto1989; Focke and Lichtenthaler 1987). Inhibition of fatty acid synthesis presumably blocks the production of phospholipids used in building new membranes required for cell growth. Broadleaf species are naturally resistant to cyclohexanedione and aryloxyphenoxy propionate herbicides because of an insensitive ACCase enzyme. Similarly, natural tolerance of some grasses appears to be due to a less sensitive ACCase (Stoltenberg 1989). An alternative mechanism of action has been proposed involving destruction of the electrochemical potential of the cell membrane, but the contribution of this hypothesis remains in question.

2$^{(B)}$ Acetolactate Synthase (ALS) or Acetohydroxy Acid Synthase (AHAS) Inhibitors

Imidazolinones, pyrimidinylthiobenzoates, sulfonylaminocarbonyltriazolinones, sulfonylureas, and triazolopyrimidines are herbicides that inhibit acetolactate synthase (ALS), also called acetohydroxyacid synthase (AHAS), a key enzyme in the biosynthesis of the branched-chain amino acids isoleucine, leucine, and valine (LaRossa and Schloss 1984). Plant death results from events occurring in response to ALS inhibition and low branched-chain amino acid production, but the actual sequence of phytotoxic processes is unclear.

3$^{(K_1)}$ Inhibitors of microtubule assembly

Benzamide, benzoic acid (DCPA), dinitroaniline, phosphoramidate, and pyridine herbicides ($K_1^{(23)}$)are examples of herbicides that bind to tubulin, the major microtubule protein. The herbicide-tubulin complex inhibits polymerization of microtubules at the assembly end of the protein-based microtubule but has no effect on depolymerization of the tubule on the other end (Vaughn and Lehnen 1991), leading to a loss of microtubule structure and function. As a result, the spindle apparatus is absent, thus preventing the alignment and separation of chromosomes during mitosis. In addition, the cell plate can not be formed. Microtubules also function in cell wall formation. Herbicide-induced microtubule loss may cause the observed swelling of root tips as cells in this region neither divide nor elongate.

4$^{(O)}$ Synthetic Auxins

Benzoic acids, phenoxycarboxylic acids, pyridine carboxylic acids, and quinoline carboxylic acids are herbicides that act similar to that of endogenous auxin (IAA) although the true mechanism is not well understood. The specific cellular or molecular binding site relevant to the action of IAA and the auxin-mimicking herbicides has not been identified. Nevertheless, the primary action of these compounds appears to affect cell wall plasticity and nucleic acid metabolism. These compounds are thought to acidify the cell wall by stimulating the activity of a membrane-bound ATPase proton pump. The reduction in apoplasmic pH induces cell elongation by increasing the activity of enzymes responsible for cell wall loosening. Low concentrations of auxin-mimicking herbicides also stimulate RNA polymerase, resulting in subsequent increases in RNA, DNA, and protein biosynthesis. Abnormal increases in these processes presumably lead to uncontrolled cell division and growth, which results in vascular tissue destruction. In contrast, high concentrations of these herbicides inhibit cell division and growth, usually in meristematic regions that accumulate photosynthate assimilates and herbicide from the phloem. Auxin-mimicking herbicides stimulate ethylene evolution which may in some cases produce the characteristic epinastic symptoms associated with exposure to these herbicides.

5$^{(C_1)}$ Inhibitors of photosynthesis at photosystem II site A

6$^{(C_3)}$ Inhibitors of photosynthesis at photosystem II site B

7$^{(C_2)}$ Inhibitors of photosynthesis at photosystem II site A; different binding behavior from group 5

All of the herbicides that fall under these three classifications kill plants by inhibiting photosystem II, however there often is not cross resistance from one class to another, hence the three classifications. Phenylcarbamates, pyridazinones, triazines, triazinones, uracils (Group 5 $^{(C_1)}$), benzothiadiazinones, nitriles, phenylpyridazines (Group 6$^{(C_3)}$) and amides and ureas (7$^{(C_2)}$), , are examples of herbicides that inhibit photosynthesis by binding to the Q_B-binding niche on the D1 protein of the photosystem II complex in chloroplast thylakoid membranes. Herbicide binding at this protein location blocks electron transport from Q_A to Q_B and stops CO_2 fixation and production of ATP and $NADPH_2$ which are all needed for plant growth. However, plant death occurs by other processes in most cases. Inability to reoxidize Q_A promotes the formation of triplet state chlorophyll which interacts with ground state oxygen to form singlet oxygen. Both triplet chlorophyll and singlet oxygen can abstract hydrogen from unsaturated lipids, producing a lipid radical and initiating a chain reaction of lipid peroxidation. Lipids and proteins are attacked and oxidized, resulting in loss of chlorophyll and carotenoids and in leaky membranes which allow cells and cell organelles to dry and disintegrate rapidly. some compounds in this group may also inhibit carotenoid biosynthesis (fluometuron) or synthesis of anthocyanin, RNA, and proteins (propanil), as well as effects on the plasmalemma (propanil) (Devine et al. 1993).

8$^{(N)}$ Inhibitors of lipid synthesis; not ACCase inhibition

Thiocarbamates and phosphorodithioates are examples of herbicides that are known inhibitors of several plant processes including: biosynthesis of fatty acids and lipids which may account for reported reductions in cuticular wax deposition. A currently viable hypothesis that may explain this mechanism of action involves the conjugation of acetyl coenzyme A and other sulfhydryl-containing biomolecules by thiocarbamate sulfoxides (Casida 1974; Fuerst 1987). The sulfoxide forms may be the active herbicides (Ashton and Crafts 1981).

9$^{(G)}$ Inhibitor of 5-enolypyruvyl-shikimate-3-phosphate synthase (EPSP)

Glycines (glyphosate) are herbicides that inhibit 5-enolpyruvylshikimate-3-phosphate (EPSP) synthase (Amrhein 1980) which produces EPSP from shikimate-3-phosphate and phosphoenolpyruvate in the shikimic acid pathway. EPSP inhibition leads to depletion of the aromatic amino acids tryptophan, tyrosine, and phenylalanine, all needed for protein synthesis or for biosynthetic pathways leading to growth. The failure of exogenous addition of these amino acids to completely overcome glyphosate toxicity in higher plants (Duke and Hoagland 1978; Lee 1980) suggests that factors other than protein synthesis inhibition may be involved. Although plant death apparently results from events occurring in response to EPSP synthase inhibition, the actual sequence of phytotoxic processes is unclear.

10$^{(H)}$ Inhibitor of glutamine synthetase

Phosphinic acids (glufosinate and bialophos) inhibit activity of glutamine synthetase (Lea 1984), the enzyme that converts glutamate and ammonia to glutamine. Accumulation of ammonia in the plant (Tachibana 1986) destroys cells and directly inhibits photosystem I and photosystem II reactions (Sauer 1987). Ammonia reduces the pH gradient across the membrane which can uncouple photophosphorylation.

11$^{(F_3)}$ Inhibitors of carotenoid biosynthesis (unknown target)

Amitrole inhibits accumulation of chlorophyll and carotenoids in the light (Ashtakala, 1989), although the specific site of action has not been determined. Precursors of carotenoid synthesis, including phytoene, phytofluene, carotenes, and lycopene accumulate in amitrole-treated plants (Barry and Pallett 1990), suggesting that phytoene desaturase, lycopene cyclase, imidazoleglycerol phosphate dehydratase, nitrate reductase, or catalase may be inhibited. Other research (Heim and Larrinua 1989), however, indicates that the histidine, carotenoid, and chlorophyll biosynthetic pathways probably are not the primary sites of amitrole action. Instead, amitrole may have a greater effect on cell division and elongation than on pigment biosynthesis. Aclonifen appears to act similar to carotenoid inhibiting/bleaching herbicides; but the exact mechanism of action in unknown.

12$^{(F_1)}$ Inhibitors of the phytoene desaturase (PDS)

Amides, anilidex, furanones, phenoxybutan-amides, pyridiazinones, and pyridines are examples of compunds that block carotenoid biosynthesis by inhibition of phytoene desaturase (Bartels and Watson 1978; Sandmann and Böger 1989). Carotenoids play an important role in dissipating the oxidative energy of singlet O_2 ($^1O_2$). In normal photosynthetic electron transport, a low level of photosystem II reaction center chlorophylls in the first excited singlet state transform into the excited triplet state (^{3}Chl). This energized ^{3}Chl can interact with ground state molecular oxygen (O_2) to form $^1O_2$. In healthy plants, the energy of $^1O_2$ is safely quenched by carotenoids and other protective molecules. Carotenoids are largely absent in fluridone-treated plants, allowing $^1O_2$ and ^{3}Chl to abstract a hydrogen from an unsaturated lipid (e.g. membrane fatty acid, chlorophyll) producing a lipid radical. The lipid radical interacts with O_2 yielding a peroxidized lipid and another lipid radical. Thus, a self-sustaining chain reaction of lipid peroxidation is initiated which functionally destroys chlorophyll and membrane lipids. Proteins also are destroyed by $^1O_2$. Destruction of integral membrane components leads to leaky membranes and rapid tissue desiccation.

13$^{(F_4)}$ Inhibitor of 1-deoxy-D-xyulose 5-phosphate synthatase (DOXP synthase)

Clomazone is the only known herbicide that falls into this class. Recent evidence suggests that clomazone is metabolized to the 5-keto form of clomazone which is herbicidally active. The 5-keto form inhibits 1-deoxy-D-xyulose 5-phosphate synthase (DOXP), a key component to plastid isoprenoid synthesis. Clomazone does not inhibit geranylgeranyl pyrophosphate biosynthesis (Croteau 1992; Weimer 1992).

14$^{(E)}$ Inhibitors of protoporphyrinogen oxidase (Protox, PPO)

Diphenylethers, *N*-phenylphthalimides, oxadiazoles, oxazolidinediones, phenylpyrazoles, pyrimidindiones, thiadiazoles, and triazolinones are herbicides that appear to inhibit protoporphyrinogen oxidase (PPG oxidase or Protox), an enzyme of chlorophyll and heme biosynthesis catalyzing the oxidation of protoporphyrinogen IX (PPGIX) to protoporphyrin IX (PPIX). Protox inhibition leads to accumulation of PPIX, the first light-absorbing chlorophyll precursor. PPGIX accumulation apparently is transitory as it overflows its normal environment in the thylakoid membrane and oxidizes to PPIX. PPIX formed outside its native environment probably is separated from Mg chelatase and other pathway enzymes that normally prevent accumulation of PPIX. Light absorption by PPIX apparently produces triplet state PPIX which interacts with ground state oxygen to form singlet oxygen. Both triplet PPIX and singlet oxygen can abstract hydrogen from unsaturated lipids, producing a lipid radical and initiating a chain reaction of lipid peroxidation. Lipids and proteins are attacked and oxidized, resulting in loss of chlorophyll and carotenoids and in leaky membranes which allows cells and cell organelles to dry and disintegrate rapidly (Duke 1991).

15$^{(K_3)}$ Inhibitors of synthesis of very long–chain fatty acids (VLCF)

Acetamide, chloroacetamide, oxyacetamide, and tetrazolinone herbicides are examples of herbicides that are inhibit very long chain fatty acid (VLCFA) synthesis (Husted et al. 1966; Böger et al. 2000). These compounds typically affect susceptible weeds before emergence, but do not inhibit seed germination.

16$^{(N)}$ Unknown site of action

Benzofuranes are known inhibitors of several plant processes including: 1) biosynthesis of fatty acids and lipids which may account for reported reductions in cuticular wax deposition, 2) biosynthesis of proteins, isoprenoids (including gibberellins), and flavonoids (including anthocyanins), and 3) gibberellin synthesis inhibition which may result from the inhibition of kaurene synthesis. Photosynthesis also may be inhibited (Gronwald 1991). The exact mechanism of action is still unknown.

17$^{(Z)}$ Unknown site of action

The organic arsenicals are place in this class. Their mechanism of action remains unknown.

18$^{(I)}$ Inhibitor of 7,8-dihydro-pteroate synthetase (DHP)

The carbamate herbicide, asulam, appears to inhibit cell division and expansion in plant meristems, perhaps by interfering with microtubule assembly or function (Fedtke 1982; Sterrett and Fretz 1975). Asulam also inhibits 7,8-dihydropteroate synthase, an enzyme involved in folic acid synthesis which is needed for purine nucleotide biosynthesis (Kidd et al. 1982; Veerasekaran et al. 1981).

19$^{(P)}$ Inhibitors of indoleacetic acid transport

Phthalamates (naptalam) and semicarbazones (diflufenzopyr) are compounds that inhibit auxin transport. These compounds inhibit polar transport of naturally occurring auxin, indoleacetic acid (IAA) and synthetic auxin-mimicking herbicides in sensitive plants. Inhibition of auxin transport causes an abnormal accumulation of IAA and synthetic auxin agonists in meristematic shoot and root regions, disrupting the delicate auxin balance needed for plant growth. When diflufenzopyr is applied with dicamba, it focuses dicamba's translocation to the meristematic sinks, where it delivers effective weed control at reduced dicamba rates and across a wider range of weed species. Sensitive broadleaf weeds exhibit rapid and severe plant hormonal effects (e.g., epinasty) after application of the mixture; symptoms are visible within hours, and plant death usually occurs within a few days. Symptomology, in sensitive annual grasses, is characterized by a stunted growth. Tolerance in corn occurs through rapid metabolism of diflufenzopyr and dicamba.

20$^{(L)}$ Inhibitor of cell wall synthesis site A

Nitriles are herbicides that inhibits cell wall biosynthesis (cellulose) in susceptible weeds (Heim et al. 1990).

21$^{(L)}$ Inhibitor of cell wall synthesis site B

Benzamides are herbicides that inhibits cell wall biosynthesis (cellulose) in susceptible weeds but the site of action appears to be different than the nitriles (Heim et al. 1990).

22$^{(D)}$ Photosystem I electron diverters

Bipyridyliums are examples of herbicides that accept electrons from photosystem I and are reduced to form an herbicide radical. This radical then reduces molecular oxygen to form superoxide radicals. Superoxide radicals then react with themselves in the presence of superoxide dismutase to form hydrogen peroxides. Hydrogen peroxides and superoxides react to generate hydroxyl radicals. Superoxides and, to a lesser extent, hydrogen peroxides may oxidize SH (sulfhydryl) groups on various organic compounds within the cell. Hydroxyl radical, however, is extremely reactive and readily destroys unsaturated lipids, including membrane fatty acids and chlorophyll. Hydroxyl radicals produce lipid radicals which react with oxygen to form lipid hydroperoxides plus another lipid radical to initiate a self-perpetuating chain reaction of lipid oxidation. Such lipid hydroperoxides destroy the integrity of cell membranes allowing cytoplasm to leak into intercellular spaces which leads to rapid leaf wilting and desiccation. These compounds can be reduced/oxidized repeatedly (Dodge 1982).

23$^{(K_2)}$ Inhibitor of mitosis

The carbamate herbicides, carbetamide, chlorpropham, and propham are examples of herbicides that inhibit cell division and microtubule organization and polymerization. The exact mechanism of inhibition is unknown.

24$^{(M)}$ Membrane disruptors (uncouplers)

Dinitrophenols (dinoterb) are herbicides that uncouple the process of oxidative phosphorylation causing almost immediate membrane disruption and necrosis.

25$^{(Z)}$ 26$^{(Z)}$ Unknown site of action

Numerous herbicides are placed in these two categories (flamprop (25) and cinmethylin; dazomet, dfenzoquat, fosamine, metham, and pelargonic acid (Group 26) because their sites of action remain unknown.

27$^{(F_2)}$ Inhibitors of 4-hydroxyhenyl-pyruvatedioxygenase (4-HPPD)

Callistemones, isoxazoles, pyrazoles, and triketones are examples of herbicides that inhibit *p*-hydroxyphenyl pyruvate dioxygenase (HPPD), which converts *p*-hydroxymethyl pyruvate to homogentisate. This is a key step in plastoquinone biosynthesis and its inhibition gives rise to bleaching symptoms on new growth. These symptoms result from an indirect inhibition of carotenoid synthesis due to the involvement of plastoquinone as a cofactor of phytoene desaturase.

28$^{(Z)}$ Unknown site of action

Several herbicides have been identified as having an unknown mode of action including the pyrazoliums (WSSA Group 26), organic arsenicals (Group 17), arylaminopropionic acids (Group 25), and other non-classified herbicides (Group 28).

30$^{(R)}$ Tyrosine Aminotransferase

Cinmethylin and methiozolin inhibit tyrosine aminotransferase via blocking conversion of 4-HPP, catalyzed by tryrosine aminotransferase (TAT), in the prenylquinone pathway, which provides plastoquinone, a cofactor of phytoene desaturase in carotenoid synthesis (Grossman et al. 2012)

NC Not classified.

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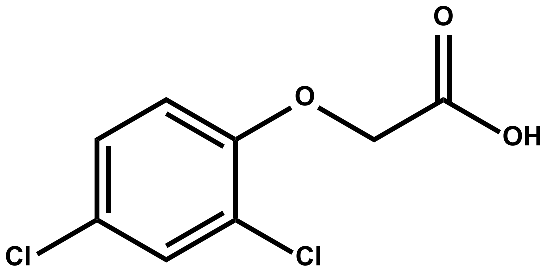
2,4-D

(2,4-dichlorophenoxy)acetic acid

CAS # Acid: 94-75-7 **$4^{(O)}$**

NOMENCLATURE

Common name: 2,4-D (BSI, ISO, WSSA)
Other name(s): Chlorophenoxy herbicides
Trade name(s): FORMULA 40*, ESTERON® 99* CONCENTRATE, HIDEP®, WEEDAR® 64, WEEDONE®, AQUA-KLEEN®, LV400 2,4-D WEED KILLER, SALVO®, SAVAGE®, WEED RHAP® A-4D, WEEDESTROY® 2,4-D LV4, DMA® 4, TRIMEC®, LANDMASTER®, NAVIGATE®.
Chemical family: phenoxy; phenoxyalkanoic acid; phenoxyacetic acid



CHEMICAL AND PHYSICAL PROPERTIES

2,4-D acid
Molecular formula: $C_8H_6C1_2O_3$
CAS Number: 94-75-7
Molecular weight: 221.0
Physical state: colorless crystals
Melting point: 138 °C
Vapor pressure (20°C): 1.4 E-7 mm Hg @25 °C
Henry's Law: 7.15 x 10^{-11} atm-m3/mol @ 25 °C
Solubility (25°C) 569 mg/L @ 20°C
Log K_{ow}: 2.81

2,4-D DMA
Common name: 2,4-D DMA
Chemical name:dimethylamine 2,4-dichlorophenoxyacetate
Molecular formula:$C_{10}H_{13}C1_2NO_3$
CAS Number: 2008-39-l
Molecular weight:266.13
Vapor pressure (20°C):Dissociates rapidly to acid
Henry's Law:Not reported.
Solubility (25°C):72.9 g/100 mL @ 20 °C
Log K_{ow}:Not reported. Dissociates rapidly to acid

2,4-D 2-ethylhexyl ester
Common name: 2,4-D 2-EHE
Chemical name:2-ethyhexyl 2,4-dichlorophenoxyacetate
Molecular formula:$C_{16}H_{22}C1_2O_3$
CAS Number:1928-43-4
Molecular weight: 333.26
Vapor pressure (20°C):3.6 E-6 mm Hg
Henry's Law:1.82 E^{-5} atm-m^3/mole
Solubility (25°C):86.7 ppb @ 20 °C
Log K_{ow}: 5.78

2,4-D choline salt
Common name:2,4-D choline salt
Chemical name:2,4-dichlorophenylacetic acid (2-hydroxyethyl trimethylammonium salt)
Molecular formula:$C_{13}H_{19}C1_2NO_4$
CAS Number:1048373-72-3
Molecular weight: 333.26
Vapor pressure (20°C):Associates rapidly to acid
Henry's Law: Not reported
Solubility (25°C):76.8% @ 25 °C
Log K_{ow}: Assoiciates rapidly to acid

HERBICIDAL USE

2,4-Dichlorophenoxyacetic acid (2,4-D) is an organic herbicide which has provided economical, selective, pre- and postemergence control of broadleaf weeds in grass crops and noncropland for the past six decades and remains a widely used herbicide throughout the world. The Environmental Protection Agency has approved 2,4-D registered products for weed control in farming, forestry, powerline maintenance, roadside brush control, aquatics, on home lawns, and for other end uses. (US EPA 2005) (9). The various forms of 2,4-D are absorbed through both the roots and leaves of most plants, especially broadleaf species.

The structure of 2,4-D is similar to that of the plant-specific hormone indole acetic acid and thus acts as a plant growth regulator. The acid is the parent compound, but many of the 2,4-D forms in use contain the amine salts, which are more water soluble than the acid, or the ester derivatives, which are readily dissolved in an organic solvent. Phenoxy herbicides play a major role in weed management when used either alone or in combination with other herbicides. Applied as a foliar spray at 10-24 ppm in water, it acts as a fruit-drop-prevention-agent in citrus. In contrast, the high majority of 2,4-D is used at higher concentrations (0.25 lbs. to 4 lbs. acid equivalent per acre) to control weeds in the crop and noncropland areas. The herbicide 2,4-D is registered for use on over 65 crops in the United States; EPA raw agricultural commodity (RAC) tolerances have been established (US EPA 2007). Also, 2,4-D is registered for numerous noncropland and aquatic uses. Applications of 2,4-D controls many broadleaf weeds including carpetweed, dandelion, cocklebur, horseweed, morningglory spp., pigweed spp., lambsquarters, ragweed spp., shepherd's-purse, and velvetleaf, with little to no activity against grasses. Aquatic weeds controlled include Eurasian water milfoil, water hyacinth, bulrush, bladderwort, and water lily.

USE PRECAUTIONS

Fire hazard: Parent acid, salts, and water-based salt formulations are non-flammable. Commercial formulations of the acid may have flash points as low as 88 C. Some ester formulations have flash points as low as 190 C (non-flammable).

Corrosiveness: Most formulated products are non-corrosive to spray equipment. Some may damage painted surfaces.

Storage stability: Most amine formulations have long storage stability and are insensitive to light and temperature. Shelf life of ester formulations varies; most retain satisfactory emulsifying properties after 3 years. Storage for amine salts: In cold zones, it is recommended to store in heated storage to prevent freezing. Storage for esters: formulated in an organic solvent, esters can be stored in colder storage. If crystallization or freezing occurs, warm the container slowly and roll to mix.

Cleaning glassware/spray equipment: Wash with water and detergent solution. Alcohol or ketone type solvents may be used for ester formulations which may be more difficult to remove from spray tanks. Ideally, equipment should not be used for application of other pesticides or fertilizers because small amounts of residues in spray equipment can be redissolved into the next load and may cause injury if applied post-emergent to sensitive broadleaf crops.

Incompatibilities: Ester formulations may be used in relatively hard water. Reduced weed control or precipitation may occur with amine formulations applied in hard water. Most amine formulations contain inhibitors to prevent precipitation in water containing up to 2000 mg/L of dissolved salts. Certain amine formulations can be used with soluble fertilizers by pre-mixing with water, but often are incompatible with liquid fertilizer. A compatibility test should be conducted with 2,4-D products before using with other pesticides or fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood but similar to that of endogenous auxin (IAA) and other auxin-type herbicides. However,2,4-D is more active than IAA and persists in the plant longer. (See page 12 for more detail).

Symptomology: Symptoms are typical of other auxin-type herbicides, and include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 2-4 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.

Absorption: Plant roots absorb polar (salt) forms of 2,4-D more readily than esters, whereas the nonpolar ester forms more rapidly penetrate foliage. A rain-free period of 4 hr. usually is adequate for uptake and effective weed control. The ester forms tend to resist washing from the leaves and are rapidly converted to the acid once inside the plant. A significant proportion of 2,4-D accumulating in cells is due to passive diffusion of the lipid-soluble protonated form of the weak acid down a concentration gradient (1). Once inside the relatively alkaline cytoplasm, the protonated acid dissociates to the anion and is consequently trapped in the symplasm because of the low solubility of the anion in membrane lipids. An active transport system also may assist in 2,4-D transport across the plasmalemma (2). Active transport of 2,4-D may occur via the same transport system as for endogenous auxin (IAA) (3).

Translocation: Transported primarily via the symplastic pathway (including the phloem) and accumulates principally at the growing points of the shoot and root. Following root uptake, 2,4-D translocates somewhat in the transpiration stream by the apoplastic pathway. Translocation generally is slower in grasses and other tolerant species. The basis for limited translocation may be the formation of immobile complexes, reduced xylem transport, and anatomical differences among species (4).

Metabolism in plants: 2,4-D metabolism in plants occurs fairly slowly. In leaves of bladder campion (*Silene vulgaris*) and lentils, at least 63% was unmetabolized after 72 h (5). Differential 2,4-D metabolism rate can account for varying 2,4-D susceptibility among species (6). 2,4-D metabolism reactions are several and can be divided into two phases (2). Phase I reactions include hydroxylation (usually involving an “NIH shift” where the #4 Cl is displaced by a hydroxyl group and moved to the #5 or #3 carbon), decarboxylation, dealkylation, and dechlorination. Phase II reactions include conjugation of amino acids, particularly glutamate and aspartate, to the side chain, and conjugation with glucose at the hydroxylated positions, followed by further oxidation to carbon dioxide.

Non-herbicidal biological properties: 2,4-D can act as a plant growth regulator, inducing rooting and blossom set when applied at low rates. It enhances the red skin coloring for red potatoes and delays preharvest dropping of some fruits. 2,4-D commonly is used in plant tissue culture as a source of auxin.

Mechanism of resistance in weeds: The precise mode of action for the auxinic herbicides such as 2,4-D is not completely understood despite their extensive use in agriculture for over six decades. Auxinic herbicide-resistant weed biotypes offer excellent model species for uncovering the mode of action as well as resistance to these compounds. Compared with other herbicide families, the incidence of resistance to auxinic herbicides is low. The relatively low incidence of resistance to auxinic herbicides has been attributed to the presence of rare alleles imparting resistance in natural weed populations, and the complex mode of action of auxinic herbicides in sensitive dicot plants. Advances in the auxin signal transduction pathway, the genetics and inheritance about the auxinic herbicide, and its relation to auxinic herbicide mode of action are being investigated. (7).

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 2,4-D is expected to be mobile (Koc = 61.7) in soil and aquatic environments. However, with its rapid dissipation characteristics, 2,4-D is not expected to move into groundwater. (8)

Transformation:

Photodegradation: Insignificant compared to aerobic soil degradation

Other degradation: 2,4-D undergoes rapid microbial breakdown in warm, moist soil.Lab DT_{50} acid values ranged from 2 to 7 days.

Persistence: Average persistence of phytotoxicity is generally 1-4 wk in warm, moist soil. Average field aerobic soil half-life is 6.2 days (8) (9).

Mobility: 2,4-D is potentially mobile, but rapid degradation in soil and removal from soil by plant uptake minimizes leaching. Dissipation studies indicate that >95% of applied 2,4-D moves <15 cm. 2,4-D has moved to 30-46 cm in sandy soils in California with heavy amounts of applied water.

Volatilization: Minor (typically negligible) losses of the acid and salts in the field (vapor pressure of 1.4×10^{-7}). Oil-soluble amines are considered least volatile. Currently registered 2-ethylhexyl and butoxyethyl ester formulations are considered low-volatile esters. However, even low-volatile esters should be used with caution around or near susceptible crops or desirable plant species.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade 2,4-D acid unless otherwise indicated.

Acute toxicity:

In acute studies 2,4-D generally has low acute toxicity (Toxicity Category III or IV) via the oral, dermal and inhalation routes of exposure. 2,4-D is not a skin irritant (Toxicity Category III or IV), the acid and salt forms are considered to be severe eye irritants (Toxicity Category I); and 2,4-D is not a dermal sensitizer (9).

Acute Oral: 2,4-D treated orally to rats. LD_{50s} as mg/kg bw/day:

- 2,4-D acid - 699
- 2,4-D DMA - 949
- 2,4-D 2-EHE - 896

Acute Dermal: Administered dermally to rabbits, 2,4-D was virtually non-toxic, LD_{50s}:

- 2,4-D acid >2000
- 2,4-D DMA 1829
- 2,4-D 2-EHE >2000

Inhalation: In acute rat inhalation studies, 2,4-D was virtually non-toxic; 2,4-D acid LC_{50} = 1.79 mg/L.

Acute Eye Irritation: 2,4-D ester forms are not eye irritants, however, the acid and salt forms are considered to be severe eye irritants.

Skin irritation: 2,4-D forms showed slight to no skin irritation.

Skin Sensitization: 2,4-D is not a skin sensitizer.

Subchronic toxicity:

90-d dietary, mouse: NOAEL 15 mg/kg/d
90-d dietary, rat: NOAEL 15 mg/kg/d
90-d dietary, dog: NOAEL 1 mg/kg/d

Chronic toxicity:

24-mo dietary, mouse: NOAEL 5 mg/kg/d
24-mo dietary, rat: NOAEL 5 mg/kg/d
12-mo dietary, dog: NOAEL 1 mg/kg/d.

Carcinogenicity: In rat and mouse subchronic and chronic studies, overall dietary NOELs were 15 and 5 mg/kg/day, respectively. 2,4-D was not carcinogenic in either rodent species, and dog, consistent with a lack of genotoxicity in *in vitro* and *in vivo* test systems. EPA classified 2,4-D as a Group D carcinogen. (9)

Developmental (Teratogenicity):

Rat: Maternal and developmental NOAEL 25 mg/kg/d; not teratogenic or embryotoxic

Rabbit: Maternal and developmental NOAEL 30 mg/kg/d; not teratogenic or embryotoxic.

Reproduction:

Rat: Parental NOAEL = 16.6 M & 40.2 F mg/kg/day (300/600 ppm); **Reproductive** NOAEL = 45.3 M & 40.2 F mg/kg/day (800/600 ppm); **Offspring** NOAEL 20.9 M & 23.3 F mg/kg (300 ppm).

Metabolism:

2,4-D is excreted unchanged in the urine as the parent acid. Once absorbed, 2,4-D is rapidly and completely excreted in urine by both rats and humans, but not dogs (11). In human studies, plasma clearance of orally administered 2,4-D was found to follow first-order kinetics with urinary excretion half-lives ranging from 5 -17 hours (11). In rats, >90% of oral doses of 30 mg/kg body weight or less were excreted in the urine within 24 hours (12).

Immunotoxicity:

2,4-D has no effect on the immune system.

Endocrine:

Completed extended one-generation reproduction toxicity study containing an endocrine module and the Endocrine Disruptor Screening Program (EDSP); current data illustrates 2,4-D is not an endocrine disruptor.

Mutagenicity:

Gene mutation: Test results negative (three tests each for the acid, 2-ethylhexyl ester, and dimethylamine salt)

Structural chromosome aberration: Test results negative

Unscheduled DNA damage/repair: Test results negative. (9)

Toxicological end points (9):

Dermal Absorption: Based on dermal absorption data from a human ^{14}C-labeled 2,4-D acid study and in harmonization with Health Canada PMRA, EPA set maximum absorption at 10%.

Dietary: The acute dietary dose and endpoint in US EPA risk assessment is NOAEL = 67 mg/kg/day for general population including infants and children. The acute dietary endpoint for female 13-49 years of age is NOAEL = 25mg/kg/day; and chronic dietary for all populations is NOAEL = 5 mg/kg/day.

Short term occupational, residential or inhalation exposure (1-30 days): Dose and Endpoint for use in risk assessment is NOAEL = 25 mg/kg/day.

Intermediate term occupational, residential or inhalation exposure: (1 to 6 months): Dose and endpoint for risk assessment is NOAEL = 15 mg/kg/day.

Long Term occupational, residential or inhalation exposure: (> 6 months): Dose and endpoint is NOAEL = 5 mg/kg/day.

Drinking Water: EPA drinking water regulations and health advisory lifetime standard for 2,4-D is 70 µg/L (ppb).

Air: NIOSH/OSHA Occupational Health Guideline for 2,4-D is 10 milligrams of 2,4-D per cubic meter of air (mg/m^3) averaged over an eight-hour shift (13).

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 2,4-D acid is prepared from 2,4-dichlorophenol and monochloroacetic acid. Salts are made by adding the appropriate amine or inorganic hydroxide to the acid. Esters are synthesized by reacting 2,4-D with the appropriate alcohols.

Purification of technical: The parent acid can be purified by recrystallization from solvents such as benzene, toluene, or xylene. Recrystallize amine salts from acetone or alcohol. 2,4-D esters are purified by vacuum distillation.

Analytical methods:

Residue – Crop and animal:

The Pesticide Analytical Manual (PAM) Vol. II lists three GC methods with microcoulometric detection and one GC method with electron capture detection (ECD). Plant commodities: GC/ECD enforcement method for plants (EN-CAS Method No. ENC-2/93). Livestock commodities: GC/ECD methods determined fat, kidney, milk and eggs. Multiresidue methods: The 10/97 edition of PDA PAM Volume I, Appendix I: Multiresidue Method Sections 402 E1 and 402 E2.

Historical: Research on 2,4-D compounds started during World War II, under wartime secrecy. Pokorny (13) described the chemical synthesis of 2,4-D in 1941. Zimmerman and Hitchcock (15) reported the potency of 2,4-D as plant hormones in 1942. Dr. E. J. Krause at the University of Chicago and Drs. P. C. Marth and J. W. Mitchell of USDA were among the earliest workers to envision the herbicidal utility of 2,4-D. English investigators included R. E. Slade, W. G. Templeman, and W. A. Secton as well as T. S. Nutman, H. G. Thornton, and J. H. Quaster, although their work was not published until 1945 due to the war. In 1944, C. L. Hamner and H. B. Tukey published on the action of 2,4-D and 2,4,5-T on bindweed. F. D. Jones described the herbicidal effects of 2,4-D in U.S. patent 2,390,941 assigned to American Chemical Paint Co. Patents on low volatile esters of 2,4-D were described in U.S. patents 2,523,227 and 2,523,228 by W. R. Mullison assigned to Dow Chemical Co. Low volatility of the butoxyethyl ester was discovered by W. W. Allen and patented under U.S. patent 2,543,397 assigned to Union Carbide. G. Templeman, and W. A. Secton as well as T. S. Nutman, H. G. Thornton, and J. H. Quaster, although their work was not published until 1945 due to the war. In 1944, C. L. Hamner and H. B. Tukey published on the action of 2,4-D and 2,4,5-T on bindweed. F. D. Jones described the herbicidal effects of 2,4-D in U.S. patent 2,390,941 assigned to American Chemical Paint Co. Patents on low volatile esters of 2,4-D were described in U.S. patents 2,523,227 and 2,523,228 by W. R. Mullison assigned to Dow Chemical Co. Low volatility of the butoxyethyl ester was discovered by W. W. Allen and patented under U.S. patent 2,543,397 assigned to Union Carbide.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama, Dow AgroSciences; PBI Gordon; Atanor; Nufarm; Industry Task Force II on 2,4-D Research Data.

Reference(s):

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2. Ashton, F. M. and T. J. Monaco. 1991. Weed Science, Principles and Practices, 3rd Ed. Wiley-Interscience, New York.
3. Rubery, P. H. 1977. Planta 135:275
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9. U.S. EPA; 2005 Reregistration Eligibility Decision (RED) 2,4-Dichlorophenoxyacetic Acid. Federal Register Notice, Vol. 70 No.151.
10. Timchalk, Charles. (2004) *Toxicology* 200:1-19.
11. Sauerhoff, M. W., et al. (1977). *Toxicology* 8, 3-11.

2,4-DB

4-(2,4-dichlorophenoxy)butanoic acid

CAS # Acid: 94-82-6
Dimethyl amine: 2758-42-1
isooctyl ester: 1320-15-6
Potassium salt: 19480-40-1
Sodium salt: 10433-59-7

4(O)

NOMENCLATURE

Common name: 2,4-DB (BSI, ISO, WSSA)

Other name(s): MB 2878; 4-(2,4-dichlorophenoxy)butyric acid (IUPAC)

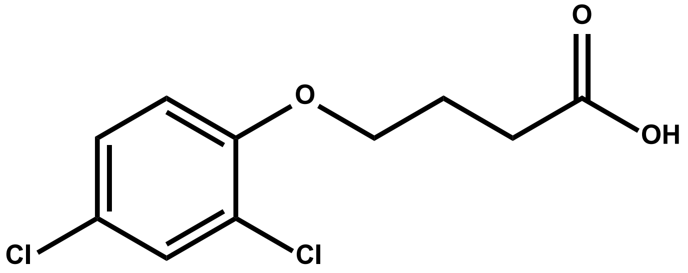
Trade name(s): BUTYRAC®; BUTOXONE®; BUTOXONE ESTER; PERSELECT

Chemical family: phenoxy; phenoxyacetic acid; phenoxyalkanoic acid

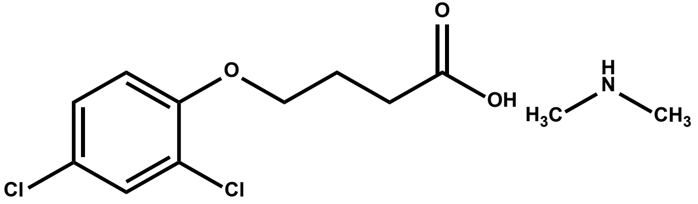
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure(s):

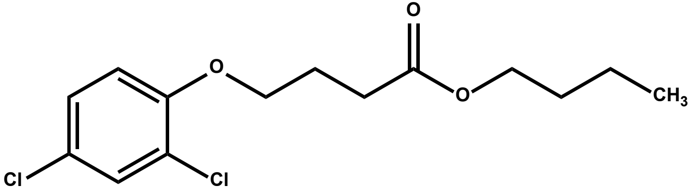
2,4-DB acid



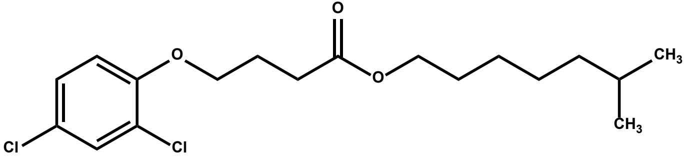
2,4-DB dimethylamine salt



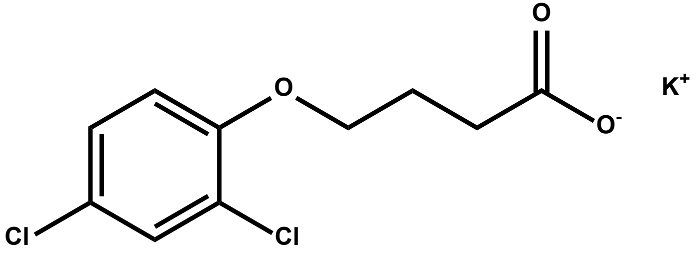
2,4-DB butyl ester



2,4-DB isooctyl ester



2,4-DB potassium salt



Molecular formula: *Acid* $C_{10}H_{10}Cl_2O_3$; *Dimethylamine (Dma) salt* $C_{12}H_{17}Cl_2NO_3$; *Isooctyl ester (Io ester)* $C_{18}H_{26}Cl_2O_3$

Molecular weight: *Acid* 249.09 g/mole; *Dma salt* 294.18 g/mole; *Io ester* 361.31 g/mole

Description: White crystalline solid, odorless when pure

Density: NA

Melting point: 120-121 C

Boiling point: NA

Vapor pressure: 1 x 10^{-5} Pa

Stability: NA

Solubility:

Acid

water 46 mg/L (25 C)
organic solvents (25 C):
acetone very soluble
ether very soluble
benzene slightly soluble
kerosene slightly soluble
diethyl ether soluble
toluene slightly soluble
ethanol very soluble

Butoxyethyl ester

water 8 mg/L (20-25 C) (7)

Dimethylamine salt

water 709,000 mg/L (20-25 C) (7)

pK_a: 4.8 (weak acid)

K_{ow}: NA

HERBICIDAL USE

2,4-DB must be applied to weed foliage and can be applied as follows: preplant or PRE at 0.14-0.25 kg ae/ha, POST at 0.0175-0.25 kg ae/ha, or POST-directed at 0.2-0.45 kg ae/ha in soybeans; at-cracking at 0.14-0.28 kg ae/ha and POST at 0.224-0.45 kg ae/ha in peanuts; POST at 0.56-1.7 kg ae/ha in seedling forage legumes and on Conservation Reserve Program (CRP) land. 2,4-DB controls several annual broadleaf weeds including pigweed spp., morningglory spp., cocklebur, common ragweed, and wild mustard. A non-ionic surfactant may be needed for maximum efficacy. In addition to application by conventional spray equipment, 2,4-DB can be applied through sprinkler irrigation systems.

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood but similar to that of endogenous auxin (IAA) and other auxin-type herbicides (more details on page 12)

Symptomology: Symptoms are typical of other auxin-type herbicides, and include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 3-5 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.

Absorption/translocation: Probably penetrates leaves readily. However, penetration rates in tolerant legume crops were slower than in certain susceptible weeds (3). 2,4-DB is translocated primarily via the symplasm (including phloem), and accumulates at the growing points. Translocation rate of 2,4-DB generally is slower than for other phenoxy herbicides, and is further reduced in tolerant species. The basis for limited translocation may be the formation of immobile complexes, reduced xylem transport, and anatomical differences among species (1).

Metabolism in plants: 2,4-DB appears to be herbicidally inactive, and must be activated by β-oxidation (cleaving two carbons from the four-carbon aliphatic side chain) in plants and soil to form 2,4-D. Conversion to 2,4-D occurs at a higher rate in 2,4-DB-susceptible species than in those tolerant to 2,4-DB. Low β-oxidase activity in tolerant species (particularly legumes) may prevent rapid conversion to 2,4-D (7). Alternatively, tolerant species may convert 2,4-DB to higher analogues by lengthening the side chain by 2-carbon units, thus yielding 2,4-dichlorophenoxyalkanoic acids with six (caproic) or ten (decanoic) carbon atoms in the aliphatic moiety (4). It is possible that both processes may be at work in 2,4-DB-tolerant species.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 440 mL/g (estimated) for the acid (2), 500 mL/g for the butoxyethyl ester (8), and 20 mL/g (estimated) for the dimethylamine salt (8)

Transformation: NA

Persistence: Average field half-life is 5 d for the acid (2), 7 d for the butoxyethyl ester (8), and 10 d (estimated) for the dimethylamine salt (8)

Mobility: NA

Volatilization: NA

weed foliage and can be applied as follows: preplant or PRE at 0.14-0.25 kg ae/ha, POST at 0.0175-0.25 kg ae/ha, or POST-directed at 0.2-0.45 kg ae/ha in soybeans; at-cracking at 0.14-0.28 kg ae/ha and POST at 0.224-0.45 kg ae/ha in peanuts; POST at 0.56-1.7 kg ae/ha in seedling forage legumes and on Conservation Reserve Program (CRP) land. 2,4-DB controls several annual broadleaf weeds including pigweed spp., morningglory spp., cocklebur, common ragweed, and wild mustard. A non-ionic surfactant may be needed for maximum efficacy. In addition to application by conventional spray equipment, 2,4-DB can be applied through sprinkler irrigation systems.

USE PRECAUTIONS

Fire hazard: Salt formulations are aqueous and nonflammable.

Corrosiveness: Non-corrosive

Storage stability: No shelf life limitations

Cleaning glassware/spray equipment: Wash with water plus detergent.

Emergency exposure: If ingested, give large quantities of water and induce vomiting.

Incompatibilities: Compatible with moderately hard water. Not intended for mixing with other pesticides.

Toxicity tests were conducted with technical grade 2,4-DB acid unless otherwise indicated.

Acute toxicity: Oral LD_{50} rat, 1960 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

Subchronic toxicity: NA

Chronic toxicity:

13-wk dietary, dog: NOEL 8 mg/kg/d

Teratogenicity: NA

Reproduction:

Rat: NOEL NA; lower ovarian weight, fewer offspring born, lower body weight, and increased pup mortality during lactation.

Mutagenicity:

Gene mutation: Ames test, negative

Wildlife:

2,4-DB acid technical: Peking duck 8-d dietary LC_{50} >1000 mg/kg

2,4-DB amine technical: Rainbow trout 96-h LC_{50} 4 mg/L; Fathead minnow 96-h LC_{50} 14 mg/L

2,4-DB isooctyl ester technical: Rainbow trout 96-h LC_{50} 4 mg/L; Fathead minnow 96-h LC_{50} 7 mg/L

Use classification: General use for all products

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React 2,4-dichlorophenol with butyrolacetone in the presence of concentrated NaOH.

Purification of technical: Recrystallize from solvents such as ethylene dichloride, etc.

Analytical methods: Total chlorine as determined by Parr Bomb may be used. The AOAC method for 2,4-D can be adapted for 2,4-DB.

Historical: The plant growth regulating properties of 2,4-DB were first reported in 1947 (5). Introduced as a herbicide by May & Baker Ltd.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Aceto Agricultural Chemicals; Agriliance; Albaugh/Agri Star; Nufarm

Reference(s):

1. Ashton, F. M. and A. S. Crafts. 1981. Mode of Action of Herbicides, 2nd ed. Wiley-Interscience, New York.
2. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
3. Hawf and Behrens. 1974. Weed Sci. 22:245.
4. Linscott and Hagin. 1970. Weed Sci. 18:197.
5. Synerholm and Zimmerman. 1947. Contrib. Boyce Thompson Inst. 14:369.
6. Tittle, F. L. et al. 1990. Plant Physiol. 94:1143.
7. Wain and Wightman. 1954. Proc. Roy. Soc. B. 142:525.
8. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

acetochlor

CAS #: 34256-82-1 **15**$^{(K_3)}$

2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl) acetamide

NOMENCLATURE

Common name: acetochlor (ANSI, BSI, ISO, WSSA)

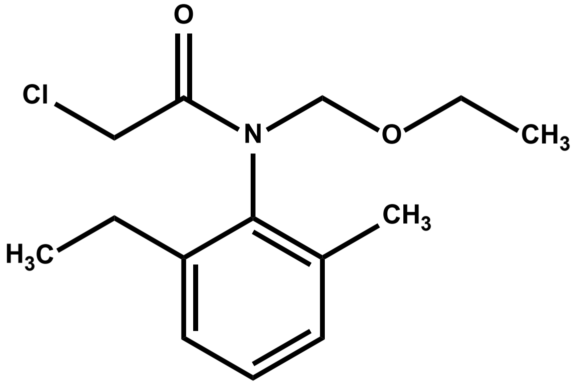
Other name(s): CP-55097; MON 097; 2-chloro-N-(ethoxymethyl)-6'-ethylacet-o-toluidide (IUPAC); 2-chloro-N-(ethoxymethyl)-6'ethyl-o-acetotoluide

Trade name(s): BREAKFREE™; BREAKFREE™ ATZ; BREAKFREE™ ATZLITE; CONFIDENCE®; CONFIDENCE® XTRA; CONFIDENCE® XTRA 5.6L; DEGREE®; DEGREE XTRA®; DOUBLEPLAY®; FIELD MASTER®; FUL TIME®; GUARDIAN®; HARNESS®; HARNESS® 20 G; HARNESS® XTRA; HARNESS® EXTRA 5.6L; KEYSTONE®; KEYSTONE® LA; SURPASS® 20 G; SURPASS® EC; TOPNOTCH™

Chemical family: acetanilide; acetamide; chloroacetamide; chloroacetanilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: acetochlor



Molecular formula: $C_{14}H_{20}ClNO_2$

Molecular weight: 269.77 g/mole

Description: Thick, oily liquid, light amber to violet, aromatic odor

Density: 1.14 g/mL (20 C); 1.11 g/mL (25 C); and 1.1 g/mL (30 C)

Melting point: <0 C

Boiling point: NA

Vapor pressure: 4.53 x 10^{-6} Pa (25 C)

Stability: Stable under normal storage conditions

Solubility:

water 223 mg/L (25 C)

organic solvents (25 C):

soluble in acetone, benzene, carbon tetrachloride, chloroform, ethanol, ether, ethylacetate, toluene

pK_a: None (non-ionizable)

K_{ow}: 300

HERBICIDAL USE

Acetochlor is applied PPI or PRE at 1.5-3.36 kg ai/ha in soybeans, and 0.93-3.36 kg ai/ha in corn. A safener is required for consistent avoidance of corn injury and is packaged with commercial acetochlor products registered for corn. Acetochlor controls most annual grasses, yellow nutsedge, and certain small-seeded broadleaf weeds.

USE PRECAUTIONS

Fire hazard: HARNESS is non-flammable; flash points are >100 C (closed cup); flash point of HARNESS PLUS is 185 C

Corrosiveness: HARNESS is slightly corrosive to mild steel.

Storage stability: Stable for at least 2 yr under normal warehouse conditions.

Cleaning glassware/spray equipment: NA

Emergency exposure: Flush eyes or skin with water. If ingested, drink water or water with activated carbon, induce vomiting 2-3 times, and drink additional water with activated carbon and a laxative; do not drink milk, grease, oil, or alcohol.

Incompatibilities: Compatible with most other pesticides and liquid fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Thought to be inhibition of very long chain fatty acid synthesis (VLCFA) (more details on page 14)

Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Susceptible monocots that do emerge appear twisted and malformed with leaves tightly rolled in the whorl and unable to unroll normally. Leaves do not emerge properly from the coleoptile and may do so underground. Broadleaf seedlings may have slightly cupped or crinkled leaves and shortened leaf midribs producing a "drawstring" effect on the leaf tip, especially under cold conditions.

Absorption/translocation: Absorbed primarily by emerging plant shoots (grass coleoptile, broadleaf hypocotyl or epicotyl), secondarily by seedling roots. Plant beyond the seedling stage readily absorb acetochlor into the roots and translocate it acropetally throughout the shoots, with primary accumulation in vegetative and less reproductive parts. Translocation in established plants is irrelevant to the mechanism of action because acetochlor is phytotoxic only to emerging seedlings.

Metabolism in plants: Acetochlor is rapidly metabolized by corn and soybean seedlings to glutathione (GSH) and homoglutathione (hGSH) conjugates, respectively (1). Plant tolerance to acetochlor depends on rates of metabolism by GSH or hGSH conjugation (2) and on endogenous levels of GSh and glutathione S-transferases (4,5).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:

K_d 0.4 mL/g for a Lintonia sand with 0.7% OM; 1.1 mL/g for a Ray silt loam with 1.2% OM; 1.6 mL/g for a Spinks sandy loam with 2.4% OM, 2.7 mL/g for a Drenner silty clay loam with 3.4% OM.

Transformation:

Photodegradation: Negligible losses

Other degradation: Degraded by microbes with negligible non-microbial degradation. Major metobolites under aerobic conditions: N-ethyoxymethyl-2'-ethyl-6'-methyl-oxanilic acid; [(N-ethoxymethyl-N-(2'ethy-6'-methyl) phenyl]-2-amino-2-oxoethyl]sulfinylacetic acid; N-ethoxymethyl)-2'-ethyl-6'-methyl-2-sulfoacetanilide.

Persistence: Generally provides 8-12 wk of weed control, but this may vary depending on soil characteristics and weather conditions. Acetochlor residues do not persist long enough to injure crops the following season.

Mobility: Acetochlor has low leaching potential in most soils. Mobility correlates well with K_d and OM content.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade acetochlor unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 2148 mg/kg; Dermal LD_{50} rabbit, 4166 mg/kg; 4-h Inhalation LC_{50} rat, >3 mg/L; Skin irritation rabbit, practically none; Skin sensitization, NA; Eye irritation rabbit, slight

HARNESS: Oral LD_{50} rat, 2676 mg/kg; Dermal LD_{50} rabbit, <5000 mg/kg; 4-h inhalation LC_{50} rat, 2.4 mg/L; Skin irritation rabbit, moderate; Eye irritation rabbit, moderate-severe

Subchronic toxicity:

90-d dietary, mouse: NOEL 2000 mg/kg; decreased body weights at 6000 mg/kg

90-d dietary, dog: NOAEL 25 mg/kg/d; mortality, reduced body weights, liver atrophy, and fatty infiltration of the renal tubules at 75 and 200 mg/kg/d; decreased food consumption and elevated SGOT at 25 mg/kg/d

21-d dermal, rabbit: Systemic NOEL 400 mg/kg/d; skin irritation at all dosages; 75% of rabbits died at 1200 mg/kg/d

Chronic toxicity:

18-d dietary, mouse: NOEL NA; MTD was exceeded at 5000 mg/kg; liver and kidney tumors at doses above the MTD; lung and uterine tumors at doses below the MTD in females; increased or decreased body weights; increased organ weights; liver damage, nephritis, and retinal degeneration

24-mo dietary, rat: Study 1, NOEL 500 mg/kg; MTD was exceeded at 5000 mg/kg; reduced body weight and food consumption, and liver necrosis at 5000 mg/kg; liver and thyroid tumors at doses above the MTD; nasal tumors at levels below the MTD, In study 2, NOEL 200 mg/kg; reduced body weight and increased nasal tumors at 1000 mg/kg

Teratogenicity:

Rat: NOEL developmental 200 mg/kg/d; not teratogenic

Rabbit: NOEL developmental 50 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 500 mg/kg; body weight decreases and reduction in viable litter sizes at 1500 and 5000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative, CHO/HGPRT, weakly positive; Mouse lymphoma, negative without activation, positive with activation

Structural chromosome aberration: Mouse micronucleus, negative; Rat dominant lethal, negative

DNA damage/repair: Primary hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, 1260 mg/kg; 8-dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Honey bee topical LD_{50}, 1715 μg/bee; Daphnia 48-h LC_{50}, 16 mg/L; Bluegill sunfish 96-h LC_{50}, 1.3 mg/L; Rainbow trout LC_{50}, 0.45 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Ethoxy methylation of the appropriate acetanilide

Purification of technical: Chromatography

Analytical methods: Gas chromatography

Historical: Acetochlor was discovered and introduced by Monsanto Company.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Adama, Agriliance; DuPont Crop Protection; Dow AgroSciences; Monsanto

Reference(s):

1. Breaux, E. J. 1986. Agric. Food Chem. 34:884.
2. Breaux, E. J. 1987. Weed Sci. 35:463.
3. Böger, P., B. Matthes, and J. Schmalfuss. 2000. Pest. Manag. Sci. 56:497-508.
4. Jablonkai and Hatzios. 1991. Pestic. Biochem. Physiol. 41:221.
5. Scarponil, L. et al. 1991. J. Agric. Food Chem. 39:2010.

acifluorfen

5-[2-chloro-4-(trifluoromethyl)phenoxyl]-2-nitrobenzoic acid

CAS # Acid: 50594-66-6
Na salt: 62476-59-9

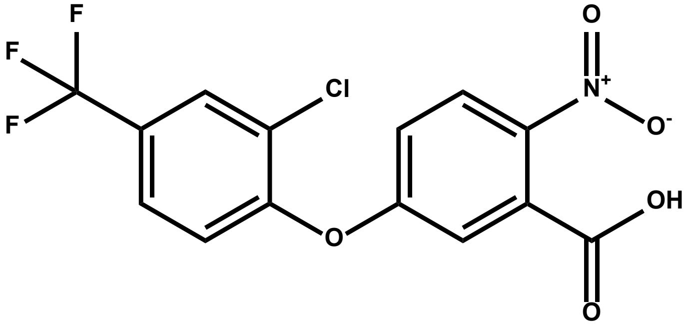
E(14)

NOMENCLATURE

Common name: acifluorfen (ANSI, BSI, ISO, WSSA)
Other name(s): acifluorfen-sodium; LS-80-1213; MC 10978; RH-6201; (Acid) 5-(2-chloro-⟨,⟨,⟨-trifluoro-p-tolyloxy)-2-nitrobenzoic acid (IUPAC); (Na salt) sodium 5-(2-chloro-⟨,⟨,⟨-trifluoro-p-tolyloxy)-2-nitrobenzoic acid (IUPAC)
Trade name(s): BLAZER®; ULTRA BLAZER®; GALAXY™; STORM®, TACKLE®
Chemical family: diphenylether; nitrodiphenylether; nitrophenylether

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
acifluorfen acid



Molecular formula: Acid $C_{14}H_7ClF_3NO_5$; Na salt $C_{14}H_6ClF_3NNaO_5$
Molecular weight: Acid 361.66 g/mole; Na salt 383.64 g/mole
Description: Acid Light tan to brown solid; Na salt Light yellow solid
Density: Acid 1.55 g/mL; Na salt 1.16-1.2 g/mL
Melting point: Acid 142 -160 C; Na salt 124-125 C
Boiling point: 217 C (1.013×10^5 Pa)
Vapor pressure: $< 1.01 \times 10^{-5}$ Pa (25 C)
Stability: Decomposes at 235 C without boiling; not hydrolyzed at pH 3-9 and 40 C; Decomposed by UV light with a half-life of ~ 110 h.
Solubility:
Acid
water, 120 mg/L (23-25 C)
organic solvents g/100 mL (25 C):
acetone 40-48
ethanol 32-39
Sodium salt
water 250,000 mg/L (25 C)
water 250,000 mg/L (25 C)
organic solvents g/100 mL (25 C)
acetone >50
ethanol >50
benzene 1\
ethyl acetate >50
carbon tetrachloride <1
n-hexane <1
chloroform <1 methanol >50
dimethyl formamide >50
methylene chloride >1
DMSO >50
xylene <1
pK_a: 3.86 ± 0.12 (weak acid)
K_{ow}: 15.6 (pH 5); < 10 (pH 7)

HERBICIDAL USE

Acifluorfen can be applied POST at 0.14-0.42 kg ai/ha in peanuts and soybeans, and POST at 0.14 kg ai/ha in rice. It controls many annual broadleaf weeds including morningglory spp., black nightshade, cocklebur, ragweed spp., jimsonweed, hemp sesbania, lambsquarters, pigweed spp., smartweed spp, wild buckwheat, and wild mustard. Early POST application at higher rates also controls several grasses including foxtail spp. And seedling johnsongrass. Surfactants or oil adjuvants increase weed control efficacy and crop injury.

USE PRECAUTIONS

Fire hazard: BLAZER is non-flammable, flash point is 210 C. Technical (Na salt) is not combustible.
Corrosiveness: Non-corrosive to equipment
Storage stability: Very stable; store above 0 C to keep from freezing
Cleaning glassware/spray equipment: Flush spray tank with water.
Emergency exposure: Flush eyes with water; get medical attention. Wash skin with soap and water. If ingested, dilute by drinking 2 glasses of water, call a physician.
Incompatibilities: Compatible with most other pesticides. Acifluorfen 0.42 kg ai/ha tank mixed with sethoxydim may anatagonize grass control. Mixing with certain insecticides may increase crop injury.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme proroporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Leaves of susceptible plants become chlorotic and then desiccated and necrotic within 1-2 d. Youngest expanded leaves of tolerant crops such as soybeans and peanuts also may show chlorosis and necrosis, especially at higher rates. Sublethal rates may produce foliar “bronzing”, usually on young expanded leaves. Droplet drift may leave bleached spots or flecks on leaves. Acifluorfen residues in soil do not affect seedling emergence.
Absorption/translocation: Readily absorbed by leaves of most species, although absorption is reduced at low relative humidity (5). Very little foliar-absorbed acifluorfen

translocates basipetally. Absorption by roots and acropetal translocation to leaves also are limited (4).

Metabolism in plants: Soybean tolerance appears to be due to rapid cleavage of the other bond by homoglutathione, producing the S-(3-carboxy-4-nitrophenyl) homoglutathione conjugate and 2-chloro-4-trifluoromethylphenol, followed by further metabolism (2). Metabolism appears to be much slower in susceptible weed species than in tolerant soybeans (4).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 113 mL/g (estimated) (7)

Transformation:

Photodegradation: Readily photodegrades with a half-life of 2-2.5 d in water and 4.5 d on soil.

Other degradation: Microbially degraded.

Persistence: Half-life is ~ 14-60 d depending on edaphic conditions. Factors that promote microbial activity enhance breakdown. Acifluorfen residues do not persist in the environment.

Mobility: Field-aged residues show negligible leaching.

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade acifluorfen Na salt unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1540 mg/kg; Dermal LD_{50} rabbit, > 2000 mg/kg; 4-h inhalation LC_{50} rat, 6.91 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, severe

BLAZER: Oral LD_{50} rat, 4790 mg/kg; Dermal LD_{50} rabbit, 3250 mg/kg; 4-h inhalation LC_{50} rat, 33 mg/L; Skin irritation rabbit, moderate, Skin sensitization guinea pig, no; Eye irritation rabbit, severe

GALAXY: Oral LD_{50} rat, > 1210 mg/kg; Dermal LD_{50} rabbit, > 2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe

STORM: Oral LD_{50} rat, > 1470 mg/kg; Dermal LD_{50} rabbit, > 2000 mg/kg; 4-h Inhalation LC_{50} rat, 5.5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe

Subchronic toxicity:

90-d dietary, rat: NOEL male 1080 mg/kg/d, female 4320 mg/kg/d

90-d dietary, dog: NOEL 5400 mg/kg/d

Chronic toxicity:

24-mo dietary, rat: NOEL 180 mg/kg/d

Teratogenicity: NA

Reproduction: NA

Mutagenicity:

Gene mutation: Ames test, negative; Mouse lymphoma, negative

Wildlife:

Bobwhite quail, oral LD_{50} 325 mg/kg, 8-d dietary LC_{50} > 5620 mg/kg; Mallard duck, oral LD_{50} 4187 mg/kg, 8-d dietary LC_{50} > 5620 mg/kg; Daphnia 48-h LC_{50} 77 mg/L; Bluegill sunfish 96-h LC_{50} 62 mg/L; Rainbow trout 96-h LC_{50} 17 mg/L.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Product analysis by gas chromatography (GC). Residue analysis by GC or high performance liquid chromatography (HPLC).

Historical: Acifluorfen was introducedas a herbicide independently by Mobil Chemical Company and by Rohm and Haas Company. It was later acquired by BASF AG.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Information source(s): BASF; United Phosphorus

Reference(s):

1. Duke, S.O. et al. 1991. Weed Sci. 39:465
2. Frear, D.S. et al. Pestic. Biochem. Physiol. 23-56.
3. Lee and Duke. 1994. Abstr. Weed Sci. Soc. Am. 34:52.
4. Ritter and Coble. 1981. Weed Sci. 29:474.
5. Ritter and Coble. 1981. Weed Sci. 29:480.
6. Stokes, J.D. et al. 1990. J. Environ. Sci. Hlth B25-55.
7. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

aclonifen

2-chloro-6-nitro-3-phenoxybenzenamine

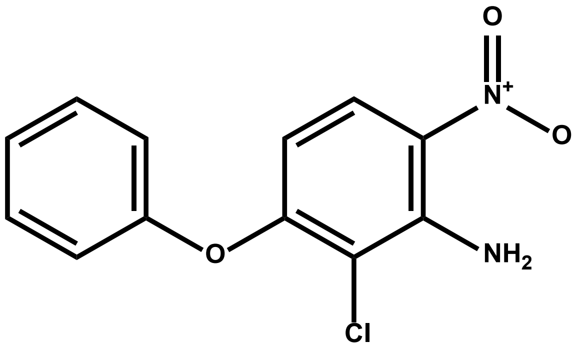
CAS #: 74070-46-5 $11^{(F_3)}$

NOMENCLATURE

Common name: aclonifen
Other name(s): CME 127; KUB 3359; 2-chloro-6-nitro-3-phenoxyaniline (IUPAC)
Trade name(s): BANDUR®; BANDREN; CARIOCA®; CHALLENGER®; FENIX®; NIKEYL®; PRODIGIO®
Chemical family: nitrodiphenylether; nitrophenylether

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:



Molecular formula: $C_{12}H_9ClN_2O_3$
Molecular weight: 264.67 g/mole
Description: Yellow crystals
Density: NA
Melting point: 81-82 C
Boiling point: NA
Vapor pressure: 9×10^{-4} Pa (20 C)
Stability: Stable to light
Solubility:
water, 2.5 mg/L (20 C)
methanol 50 mg/L
hexane 4.5 mg/L
toluene 390 mg/L (20 C)
pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

Aclonifen can be used pre-emergence in several crops including corn, winter wheat, potatoes, and several vegetables.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: NA
Storage stability: Stable under normal storage conditions.
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Appears to act similar to carotenoid-inhibiting bleaching herbicides; exact mechanism is unknown.(For more detail see page 13)
Symptomology: Growth of susceptible plants is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by slow, general foliar chlorosis and necrosis.
Absorption/translocation: Moves in both the xylem and phloem.
Metabolism in plants: Hydroxylation occurs on both benzene rings. Half-life is approximately 2 wk.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: None known

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 5318-12164 mL/g
Transformation: NA
Persistence: DT_{50} 36-80 d (22 C)
Mobility: Unlikely to leach: -0.13 < GUS <0.64
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade aclonifen unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >4.83 mg/L (max, attainable conc.); Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, none.
Subchronic toxicity:
90-d dietary, rat: NOEL 28 mg/kg/d
Chronic toxicity:
6-mo dietary, dog: NOEL 3 mg/kg/d
Mutagenicity:
Gene mutation: Ames test, negative
Wildlife:
Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Honey bee topical LD_{50}, >100 ∝g/bee; Daphnia 48-h LC_{50}, >100 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L; Channel catfish 96-h LC_{50}, >100 mg/L
Use classification: General use; EPA Class IV

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Roberts, T. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.

acrolein

2-propenal

CAS #: 107-02-8

NC

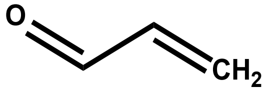
NOMENCLATURE

Common name: acrolein (WSSA)
Other name(s): acrylaldehyde or prop-2-enal (IUPAC)
Trade name(s): MAGNACIDE® H
Chemical family: None generally accepted

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

acrolein



Molecular formula: C_3H_4O
Molecular weight: 56.06 g/mole
Description: Purified dry acrolein is highly unstable and is virtually unavailable. Available "technical" is a 97% w/w aqueous solution (actual concentration varies from 92-97% w/w), a colorless liquid with a pungent odor. The aqueous technical is identical to the formulated product (MAGNACIDE H HERBICIDE).
Density: 0.847 g/mL (15.6 C) *(97% w/w aqueous technical)*
Melting point: 86.95 C *97% w/w aqueous technical*
Boiling point: 52.69 C *97% w/w aqueous technical (comment: boiling point is lower than melting point; must be measured at different pressue?)*
Vapor pressure: 8.1 x 10^3 Pa (10 C); 28 x 10^3 Pa (20 C); 32 x 10^3 Pa (25 C); 43 x 10^3 Pa (30 C); and 92.3 x 10^3 (50 C) *(97% w/w aqueous technical)*
Stability: Polymerizes in the presence of acid or base (*97% w/w aqueous technical)*
Solubility:

97% w/w aqueous technical

water 237,628 mg/L acrolein technical (25 C), and 7% w/w water in acrolein technical (20 C)

organic solvents (25 C):

acetone miscible
benzene miscible
ethanol miscible
ether miscible
hydrocarbons miscible
methanol miscible

pK_a: None (non-ionizable)
K_{ow}: *97% w/w aqueous technical* 1.10

HERBICIDAL USE

Acrolein can be applied at 1-15 mg/L (injected below the water surface) for control of submersed and floating aquatic weeds and algae in irrigation canals. It is toxic to fish and wildlife and must be kept out of lakes, streams, and ponds. Emergent weeds are not controlled at recommended rates. Floating weeds such as *Pistia*, *Eichornia*, and *Jussiaea* spp. are controlled only when acrolein concentration is maintained at 15 mg/L for an extended period.

USE PRECAUTIONS

Fire hazard: MAGNACIDE H HERBICIDE is extremely flammable; flash point is -25 C
Corrosiveness: MAGNACIDE H HERBICIDE is corrosive to skin.
Storage stability: MAGNACIDE H HERBICIDE can polymerize in the presence of strong acid or alkali with force sufficient to rupture storage containers; must be stored in darkness, under nitrogen; stable in an 18-mo storage test

Cleaning glassware/spray equipment: Clean with water and detergent
Emergency exposure: If ingested, do not induce vomiting; drink large quantities of milk, egg whites, gelatin, or, if these are not available, water; seek medical treatment. Treatment for circulatory shock, respiratory depression, and convulsion may be needed. Irritates eyes and open wounds. Flush eyes with water. Severe cases of exposure to vapor may progress to pulmonary edema.
Incompatibilities: Many chemical and equipment incompatibilities (see product label and safety manual)

BEHAVIOR IN PLANTS

Mechanism of action: Acrolein is a general cell toxicant that reacts with sulfhydryl groups on a variety of biomolecules, destroying enzymes and disrupting plant metabolic systems.
Symptomology: Weeds become flaccid within a few h, followed by gradual chlorosis and tissue disintegration.
Absorption/translocation: Absorbed readily by aquatic plants, but poorly by terrestrial plants
Metabolism in plants: Metabolized in lettuce to water-soluble conjugates
Non-herbicidal biological properties: Acrolein is a general biocide
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil
K_{oc}: Average is 0.5 mL/g (1)
Transformation: Acrolein in water can be oxidized to acrylic acid, hydrolyzed to form 3-hydroxypropanal, or reduced to allyl alcohol. Furthert oxidative or reductive reactions in conjunction with decarboxylation produces oxalic acid and CO_2. Hydrolysis appears to be an early step in degradation in aerobic and anerobic water and sediment. Hydrolysis half-life in laboratory water was 3.5 d (pH 5), 1.5 d (pH 7), and 4 h (pH 10). Half-life was 4.2 h for aerobic and 11 d for anaerobic soil metabolism.
Persistence: Acrolein persistence in aquatic environments is affected by water temperature and pH; half-life in water is 150 h (pH 5), 120-180 h (pH 7), and 5-40 h (pH 9)

Field experiments: Half-life was 5.5 h in an Idaho study. Half-life was 7.5 h in a non-weed canal and 10 h in a weeded canal in California. Half-life was 8.3 h in an Arizona study. Half-life was 10.2 h in a pump canal in

Washington.

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade acrolein (97% w/w aqueous) unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 29 mg/kg; rabbit, 7.1 mg/kg; male mouse, 13.9 mg/kg; female mouse, 17.7 mg/kg; Dermal LD_{50} rabbit, 231 mg/kg; 4-h inhalation LC_{50} rat, 8.3 mg/L, 1-h inhalation LC_{50} rat, 26 mg/L; Skin irritation rabbit, yes; Skin sensitization, NA; Eye irritation rabbit, yes

Subchronic toxicity:

90-d dietary, rat: NOEL NA; no effects at up to 5 mg/kg/d; no adverse effects when fed water containing 200 mg/L

21-d dermal, rabbit: NOEL NA; slight to moderate depression in body weight and food consumption; gross skin lesions more severe at higher rates (max. dose 63 mg/kg/d); increased incidence of histopathologic lesions

Chronic toxicity:

24-mo dietary, rat: NOEL NA; increased mortality but no increased incidence of tumors or lesions at up to 2.5 mg/kg/d

18-mo dietary, mouse: NOEL NA; increased mortality but no increased incidence of tumors or lesions at up to 4.5 mg/kg/d

12-mo dietary, dog: NOEL NA; blood chemistry changes but no increased incidence of tumors or lesions at up to 2 mg/kg/d

Teratogenicity:

Rat: NOEL NA; not teratogenic at levels causing maternal toxicity (max. dose 10 mg/kg/d)

Rabbit: NOEL NA; not teratogenic at levels causing maternal toxicity (max. dose 2 mg/kg/d)

Reproduction:

Rat: NOEL NA; no reproductive toxicity at up to 7.2 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative with or without metabolic activation; CHO/HGPRT, negative with or without metabolic activation

Structural chromosome aberration: CHO/SCE, negative; Rat bone marrow, negative

Mammalian cell transformation: Mouse fibroblasts (C3H/10T/2), negative

Wildlife:

Acrolein aqueous technical: Bobwhite quail oral LD_{50}, 19 mg/kg; Mallard duck oral LD_{50}, 30.2 mg/kg; Daphnia 48-h LC_{50}, 0.022 mg/L; Bluegill sunfish 24-h LC_{50}, 0.024 mg/L; Rainbow trout 24-h LC_{50}, .024 mg/L; Shiner 24-h LC_{50}, 0.04 mg/L; Mosquito fish 24-h LC_{50}, 0.39 mg/L; Mysid shrimp, 48-h LC_{50}, 0.5 mg/L, NOEC, 0.036 mg/L; Oyster 48-h EC_{50}, 0.18 mg/L, NOEC 0.032 mg/L; Sheepshead minnow LC_{50}, 0.57 mg/L, NOEC 0.13 mg/L

Use classification: Restricted use because of toxicity to fish and other aquatic organisms

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Commercially prepared through vapor phase oxidation of propylene with air or oxygen in the presence of a catalyst.

Purification of technical: Distillation through a 40-plate Oldershaw column at a 40:1 reflux ratio. The water azeotrope center is removed by azeotropic redistillation with diethyl ether. Acrolein is again refractioned to first remove the ether and then to obtain a center weight of high purity anhydrous acrolein. Light and oxygen must be excluded from the distillations. The finished sample must be refrigerated.

Analytical methods: Residues in water are determined by conversion to the 2,4-dinitrophenylhydrazone and colorimetry of this derivative.

Historical: Fifteen years after Wohler's transformation of ammonium cyanate into urea in 1828, Redtenbacher (3) reported the discovery of acrolein from the dry distillation of fats and glycerol. In 1898, Deniges (2) isolated acrolein as a decomposition product from a propylenemercuric sulfate complex in the first preparation of the unsaturated aldehyde from a petroleum-derivable hydrocarbon. With the commercial development of aliphatic organic chemicals during the 1930s, acrolein production from petroleum products was improved. Shell Co. developed a process for acrolein production and obtained patents 2,042,220, 2,959,476, and 2,978,475 in 1948.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Baker

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Deniges, G. 1898. Compt. Rend. 126:1147.
3. Redtenbacher, J. 1843. Ann. 47:114.

alachlor

CAS #: 15972-60-8 **15$^{(K_3)}$**

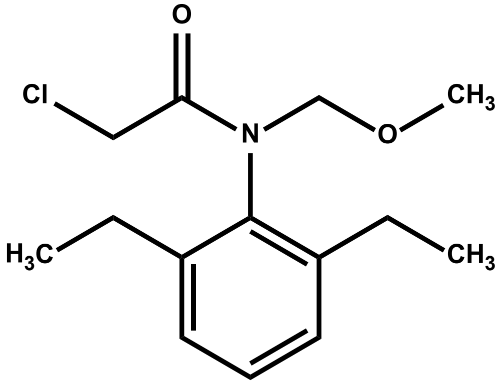
2-chloro-*N*-(2,6-diethylphenyl)-*N*-(methoxymethyl) acetamide

NOMENCLATURE

Common name: alachlor (ANSI, BSI, ISO, WSSA)
Other name(s): alachlore; CP-50144; ⟨-chloro-2',6'-diethyl-*N*-(methoxymethyl)acetanilide; 2-chloro-2',6'-diethyl-*N*-methoxymethylacetanilide (IUPAC); 2-chloro-2',6'-diethyl-*N*-(methoxymethyl)acetanilide
Trade name(s): ADAR®; ALAGAM®; ALAGAN; ALACHLOR; ALATOX480; BULLET®; CHIMICLOR; FREEDOM®; INTRRO®; LARIAT®; LASSO®; LASSO II®; LASSO MICRO-TECH®; MICRO-TECH; LAZO; RAMBO; SWIFT®
Chemical family: acetanilide; acetamide; chloroacetamide; chloroacetanilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *alachlor*



Molecular formula: $C_{14}H_{20}ClNO_2$
Molecular weight: 269.77 g/mole
Description: Cream to wine-red colored solid; odorless
Density: 1.13 g/mL (25 C)
Melting point: 39.5-41.5 C
Boiling point: 100 C (2.67 Pa) and 135 C (39.99) Pa
Vapor pressure: 2.13 x 10^{-3} Pa (25 C); 2.67 Pa (110 C)
Stability: Stable to UV light; slowly decomposes at 105 C; hydrolyzed under strongly acid or alkaline conditions
Solubility:
water 200 mg/L (20 C), 242 mg/L (25 C)
organic solvents (25 C):
acetone soluble
benzene soluble
chloroform soluble
ether soluble
ethanol soluble
ethyl acetate soluble
heptane slightly soluble

pK_a: None (non-ionizable)
K_{ow}: 794

HERBICIDAL USE

Alachlor can be applied as follows: early preplant, no-till at 2.5-4.2 kg ai/ha or PPI, PRE, or early POST at 1.7-6.7 kg ai/ha in corn; PPI or PRE at 1.7-3.4 kg ai/ha in grain sorghum; PPI or PRE at 2-3.36 kg ai/ha in soybeans; PPI, PRE, or at-cracking at 3.4-4.5 kg ai/ha in peanuts; PPI at 2.2-3.4 kg ai/ha in drybeans; PPI at 2.2-3.4 kg ai/ha and PRE at 1.7-3.4 kg ai/ha in lima beans (green); and PRE-directed at 4.5 kg ai/ha in woody ornamentals. Alachlor controls yellow nutsedge, many annual grasses such as barnyardgrass, crabgrass spp., foxtail spp., panicum spp., goosegrass, and certain broadleaf weeds such as galinsoga, lambsquarters, purslane, and black nightshade.

USE PRECAUTIONS

Fire hazard: EC formulations (FREEDOM, LASSO) are combustible. Alachlor technical along with granular and SC formulations are dry or aqueous and are not combustible.
Corrosiveness: LASSO, LARIAT, BULLET, and FREEDOM are corrosive to steel and black iron, but are not corrosive to #316 and #304 stainless steel and aluminum. MICRO-TECH is corrosive to stainless steel.
Storage stability: Indefinitely stable under normal storage conditions.
Cleaning glassware/spray equipment: Wash with detergent.
Emergency exposure: If ingested, induce vomiting
Incompatibilities: Compatible with water of <1000 mg/L hardness and with most liquid fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Thought to be inhibition of very long chain fatty acid synthesis (VLCFA) (more details on page 14)
Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Susceptible monocots that do emerge appear twisted and malformed with leaves tightly rolled in the whorl and unable to unroll normally. Leaves do not emerge properly from the coleoptile and may do so underground. Broadleaf seedlings may have slightly cupped or crinkled leaves and shortened leaf midribs producing a "drawstring" effect on the leaf tip.
Absorption/translocation: Absorbed primarily by emerging plant shoots (grass coleoptile, broadleaf hypocotyl or epicotyl), secondarily by seedling roots. Plants beyond the seedling stage readily absorb alachlor into the roots and translocate it acropetally throughout the shoots, with primary accumulation in vegetative and less in reproductive parts. Translocation in established plants is irrelevant to mechanism of action because of alachlor is phytotoxic only to emerging seedlings.
Metabolism in plants: Detoxified by conjugation with gluthathione (GSH) or, possibly in certain legumes, with homoglutathione. Conj Involvement of GSH transferase is uncertain. GSH conjugate is subsequently metabolized to the malonylcysteine conjugate.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:

K$_{oc}$: ranges from 43-209 mL/g

Transformation:

Photodegradation: Half-life is 80 d on soil and >239 d in water; minor contributions to losses in the field.

Other degradation: Alachlor degradation is sterilized soil is negligible. Major soil metabolites formed by microbial degradation are: 2,6-diethyl-*N*-methoxy-methyloxanilic acid; 2′,6′-diethyl-*N*-methoxymethyl-2-sulfoacetanilide; 2,6-diethyloxanilic acid; 2′,6′-diethyloxanilic acid; 2′,6′-diethyloxanilic acid; 2′,6′-diethyloxanilic acid; 2′,6′-diethyl-2-sulfoacetanilide; 2′,6′-diethyl-2-hydroxy-*N*-methoxymethyl-acetanilide; 2′,6′-1-diethyl-*N*-methoxymethyl-2-methylsulfinyl acetanilide. Half-life in aerobic soil is 6.1-15.8 d, but 4.5 d in anaerobic (aquatic) conditions.

Persistence: Average field half-life is 21 d. Alachlor generally provides 6-10 wk of weed control, but this varies with soil characteristics and weather conditions. Alachlor residues do not persist long enough to injure crops the following season.

Mobility: Low to moderate mobility in soil

Volatilization: Low losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade alachlor unless otherwise indicated.

Acute toxicity:

Oral LD$_{50}$ rat, 930-150 mg/kg; rabbit, 1740 mg/kg; mouse, 1100 mg/kg; Dermal LD$_{50}$ rabbit, 13,300 mg/kg; 4-h inhalation LC$_{50}$ rat, >5.1 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, none

LASSO: Oral LD$_{50}$ rat, 2000 mg/kg; Dermal LD$_{50}$ rabbit, 7800 mg/kg; 4-h inhalation LC$_{50}$ rat, >6.51 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe

LASSO II: Oral LD$_{50}$ rat, >5010 mg/kg; Dermal LD$_{50}$ rabbit, >5010 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, slight

MICRO-TECH: Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rabbit, >5000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, none

PARTNER: Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rabbit, >5000 mg/kg; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, moderate

BRONCO: Oral LD$_{50}$ rat, 3152 mg/kg; Dermal LD$_{50}$ rabbit, >5000 mg/kg; Skin irritation rabbit, moderate; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe

BULLET: Oral LD$_{50}$ rat, 8900 mg/kg; Dermal LD$_{50}$ rabbit, >5000 mg/kg; 4-h inhalation LC$_{50}$ rat, >1.1 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

FREEDOM: Oral LD$_{50}$ rat, 2650 mg/kg; Dermal LD$_{50}$ rabbit, >5000 mg/kg; 4-h inhalation LC$_{50}$ rat, >3.9 mg/L; Skin irritation rabbit, severe; Skin sensitization guinea pig, no; Eye irritation rabbit, severe

LARIAT: Oral LD$_{50}$ rat, 4400 mg/kg; Dermal LD$_{50}$ rabbit, >5000 mg/kg; Skin irritation rabbit, severe; Skin sensitization guinea pig, yes; Eye irritation rabbit, moderate **Subchronic toxicity:**

6-d dietary, dog: NOEL 5 mg/kg/d; mortality, reduced body weight gain, and liver toxicity

3-wk dermal, rabbit: Systemic NOEL 1000 mg/kg/d; skin irritation and increased pituitary weights

1-mo inhalation study, rat: NOEL <0.06 mg/L; reduced body weight, sensory irritation, and increased liver weight

Chronic toxicity:

24-d dietary, mouse: NOEL 25 mg/kg/d

18-mo dietary, mouse: NOEL 26 mg/kg/d; decreased body weight gain and increased liver and kidney weights; not oncogenic

25-mo dietary, rat: NOEL 25 mg/kg/d; decreased survival, body weight loss, ocular toxicity, nasal inflammation, liver toxicity, and liver tumors at 126 mg/kg/d (high dose). The high dose exceeded the MTD

12-mo dietary, dog: NOEL 1 mg/kg/d; decreased body weight; mild liver toxicity, diarrhea, and hemolytic anemia

Teratogenicity:

Rat: NOEL 150 mg/kg/d; not teratogenic

Rabbit: NOEL developmental 150 mg/kg/d; maternal 100 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 30 mg/kg/d; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; *E. coli*, negative; *B. subtilis* REC, negative; CHO/HGRT, negative

Structural chromosome aberration: Mouse dominant lethal, negative; *In vivo* rat bone marrow, negative; *In vivo* rat micronucleus, negative

DNA damage/repair: *In vitro* rat UDS, negative; *In vivo* UDS, equivocal (not a clear positive)

Wildlife: Bobwhite quail oral LD$_{50}$, 1536 mg/kg, 5-d dietary LC$_{50}$, >5620 mg/kg; Mallard duck 5-d dietary LC$_{50}$, >5620 mg/kg; Daphnia 48-h LC$_{50}$, 10 mg/L; Bluegill sunfish 96-h LC$_{50}$, 2.8 mg/L; Rainbow trout 96-h LC$_{50}$, 5.3 mg/L; Channel catfish 96-h LC$_{50}$, 2.1 mg/L; Fathead minnow 96-h LC$_{50}$, 5 mg/L; Crayfish 96-h LC$_{50}$, 320 mg/L

LASSO: Daphnia 48-h LC$_{50}$, 22 mg/L; Bluegill sunfish 96-h LC$_{50}$, 6.2 mg/L; Rainbow trout 96-h LC$_{50}$, 3.7 mg/L

LASSO II: Bobwhite quail oral LD$_{50}$, >2510 mg/kg; 5 d dietary LC$_{50}$, >5620 mg/kg

MICRO-TECH: Bobwhite quail oral LD$_{50}$, >2510 mg/kg; 5-d dietary LC$_{50}$, >9094 mg/kg; Mallard duck 5-d dietary LC$_{50}$, >9094 mg/kg; Honeybee topical LD$_{50}$, >100 ∝g/bee; Daphnia 48-h EC$_{50}$, >1 mg/L; Bluegill sunfish 96-h LC$_{50}$, 270 mg/L; Rainbow trout 96-h LC$_{50}$, 130 mg/L

BRONCO: Daphnia 48-h EC$_{50}$, 50 mg/L; Bluegill sunfish 96-h LC$_{50}$, 13 mg/L; Rainbow trout 96-h LC$_{50}$, 7.5 mg/L

Use classification: Restricted Use due to oncogenicity in rat

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Methoxy methylation of the appropriate acetanilide

Purification of technical: Crystallization at 30 C

Analytical methods: GC with electron capture detection or mass spectrometry.

Historical: Herbicidal activity of the chloroacetamides was discovered in 1952 by Monsanto (2). Alachlor was first reported in 1966 (3) and commercialized as LASSO in 1969 by Monsanto. It is protected under U.S. patents 3,442,945, 3,547,620 and others.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Adama, Monsanto; Micro Flo;

Reference(s):

1. Böger, P., B. Matthes, and J. Schmalfuss. 2000. Pest. Manag. Sci. 56:497-508.
2. Hamm, P. C. 1974. Weed Sci. 22:541.
3. Husted, R. F. et al. 1966. Proc. North Cent. Weed Control Conf. 44.

alloxydim

CAS #: 55634-91-8

1$^{(A)}$

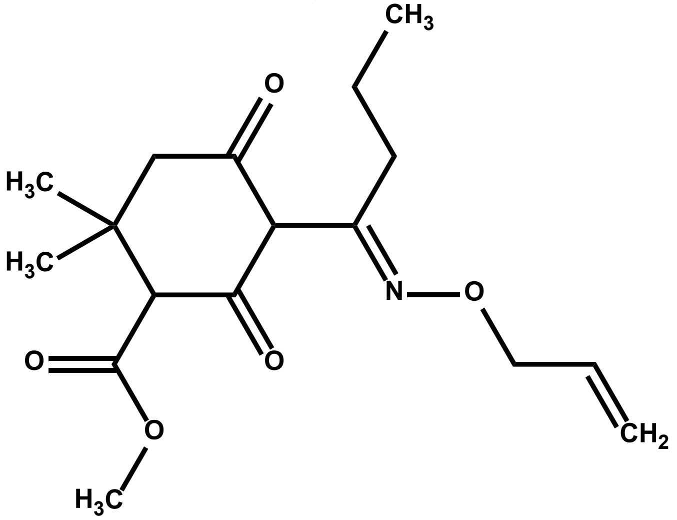
methyl 2,2-dimethyl-4,6-dioxo-5-[(1E)-1[(2-propenyloxy)imino]butyl]cyclohexanecarboxylate

NOMENCLATURE

Common name: alloxydim (ISO-approved)
Other name(s): NP-48Na; methyl (1RS)-3-[(E)-1-(allyloxyimino)butyl]-4-hydroxy-6,6-dimethyl-2-oxocyclohex-3-enecarboxylate (IUPAC)
Trade name(s): CLOUT®; FERVIN®; KUSAGARD®; MONOLOX®
Chemical family: cyclohexanedione; cyclohexane-dione oxime; cyclohexenone; cyclohexene oxime

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: alloxydim



Molecular formula: $C_{17}H_{25}NO_5$
Molecular weight: 323.4 g/mole
Description: Colorless crystals
Density: NA
Melting point: NA
Boiling point: 185.5 C (2)
Vapor pressure: <1.33 x 10^{-4} Pa (25 C)
Stability: Stable when dry, but very hygroscopic
Solubility: In water, >2,000,000 mg/L (20 C)
pK$_a$: 4.1 (weak acid)
K$_{ow}$: log K_{ow} = -0.02

HERBICIDAL USE

Alloxydim is used for POST control of annual and perennial grass weeds in sugar beet, vegetables and broadleaf crops at 0.5 to 1 kg ai/ha.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Cleaning glassware/spray equipment: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)
Symptomology: Growth ceases within a few days of application with meristematic regions affected first. Leaf chlorosis and eventually necrosis develop within 1-3 wk of application. Leaf sheaths become brown and flaccid attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.
Absorption/translocation: Rapidly absorbed into roots and leaves; translocated predominately in the phloem
Metabolism in plants: Degraded very rapidly on the leaf surface via photochemical reactions; breakdown is so rapid that it is possible that a degradation product is the active herbicide
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Similar to other ACCase-resistant weeds

BEHAVIOR IN SOIL

Sorption:
K$_{oc}$: 7 mL/g
Transformation:
Photodegradation: Aqueous photolysis $DT_{50,}$ 0.22 d; very rapid
Other degradation: Neutral hydrolysis DT_{50}, 15 d; Water/sediment DT_{50}, 49 d; hydrolysis followed by rearrangement to oxazoles is expected
Persistence:
Field experiments: DT_{50} of 2-10 d
Mobility: GUS index, 4.10; high leachability
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade alloxydim unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, > 2322 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg
Subchronic toxicity:
2-y dietary, rat: NOEL = 100 mg/kg
Mutagenicity: Non-mutagenic
Wildlife:
Japanese quail oral LD_{50}, >2970 mg/kg; Honey bee, non-toxic; Carp 96-h LC_{50}, 2600 mg/L; Rainbow trout 96-h LC_{50}, 200 mg/L
Use classification: WHO Class III, EPA Class III

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1. Roberts, T. 1998. Metabolic Pathways of Agrochemcals. Vol. 1 Royal Society of Chemistry.
2. Yoshii, K. and Y. Tonogai. 2004. J. Health Sci. 50:142-147.

ametryn

CAS #: 834-12-8

$5^{(C_1)}$

N-ethyl-*N'*-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: ametryn

Other name(s): ametryne (BSI); G-34162; ametrin; ametrine; ametrina; *N*^{2}-ethyl-*N*^{4}-isopropyl-6-methylthio-1,3,5-triazine-2,4-diamine (IUPAC); 2-(ethylamino)-4-(isopropylamino)-6-(methylthio)-*s*-triazine

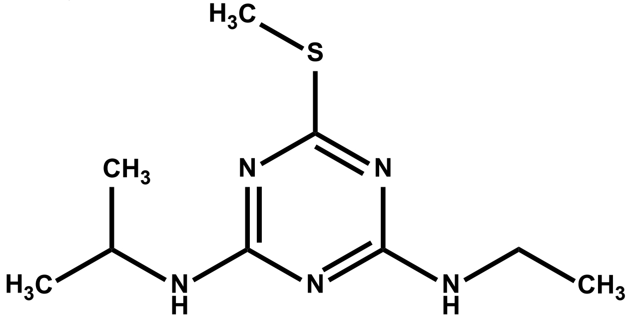
Trade name(s): GESAPAX; EVIK®; TRINATOX D; X-SIPAX; SEGARD

Chemical family: methylthio-*s*-triazine; methylthio triazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

ametryn



Molecular formula: $C_9H_{17}N_5S$

Molecular weight: 227.33 g/mole

Description: White crystalline solid

Density: 1.19 g/mL

Melting point: 84-85 C

Boiling point: NA

Vapor pressure: 2.53×10^{-5} Pa (10 C); 1.12×10^{-4} Pa (20 C); 3.60×10^{-4} Pa (25 C); 4.40×10^{-4} Pa (30 C); 1.60×10^{-3} Pa (40 C); 5.20×10^{-3} Pa (50 C); Henry's Law constant, 4.09×10^{-9} atm m^3/mole

Stability: Decomposed by UV light; high temperature decomposition unknown; hydrolyzes to the 6-hydroxy analogue with 50% loss (calculated) at 20 C in 32 d (pH 1) to >200 d (pH 13)

Solubility:

water 200 mg/L (pH 7.1, 22 C)
organic solvents g/100 mL (20 C):
acetone 56.9
dichloromethane 61.4
n-hexane 1.4
methanol 51.6
n-octanol 24.2
toluene 46

pK_a: 4.1 (20 C) (weak base)

K_{ow}: 427 (pH 7, 25 C)

HERBICIDAL USE

Ametryn can be applied as follows: PRE or POST at 1.8-9 kg ai/ha as single or multiple applications in bananas and plantains; POST-directed at 0.67-2.2 kg ai/ha in field corn, sweet corn, and popcorn; PRE at up to 9 kg ai/ha in pineapple followed by POST applications at 2.2 kg ai/ha; PRE at 2.2-9 kg ai/ha or POST-directed at 0.45-1.3 kg ai/ha in sugarcane; and POST at 0.67-2.2 kg ai/ha on non-crop land. Ametryncontrols several annual grass and broadleaf weeds including fall panicum, giant foxtail, shattercane, pigweed spp., velvetleaf, smartweed spp., and many other troublesome species in semi-tropical and tropical crops.

USE PRECAUTIONS

Fire hazard: The product EVIK 80W is non-flammable and has low electrical conductivity

Corrosiveness: The product EVIK 80W is non-corrosive.

Storage stability: The product EVIK 80W is stable over several years of cool, dry storage; slowly decomposed by UV light.

Cleaning glassware/spray equipment: Wash with water

Emergency exposure: Rinse eyes with water. Wash skin with soap and water. If ingested, drink 1-2 glasses of water and induce vomiting or lavage stomach; give a saline laxative and supportive therapy. Ingestion may cause nausea, vomiting, abdominal distress, or diarrhea. No specific antidote is available, but activated charcoal at 5 mg/kg body weight in a water suspension may help inactivate the herbicide.

Incompatibilities: Compatible with most other pesticides and fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)

Symptomology: Symptoms in susceptible plants begin with interveinal chlorosis of the leaves and yellowing of leaf margins within 2-3 d, followed by further chlorosis and necrosis. Browning of leaf tips can occur. Older tissue generally shows more injury than new growth. Root growth is not affected.

Absorption/translocation: Readily absorbed by foliage and roots. Foliar penetration is rapid, especially when a surfactant is added, minimizing removal from foliage by rain. Ametryn translocates acropetally predominately through the xylem from roots into foliage, accumulating in apical meristems and leaf margins.

Metabolism in plants: Readily metabolized in tolerant plants by oxidation of the methylthio group to the hydroxy derivative or by conjugation with glutathione. These reactions constitute the major detoxification pathways in most tolerant crops and weeds. Hydroxyametryn is further degraded by side chain *N*-dealkylation, producing amino groups which are converted to hydroxy groups by deamination.

Non-herbicidal biological properties: Ametryn has been used as a potato vine desiccant due to its rapid action.

Mechanism of resistance in weeds: Over 60 species worldwide have developed triazine-resistant biotypes. Those studied at the genetic level have an altered *psbA* gene coding for a glycine in place of a serine on the D1 protein on which the ametryn binding site is located. Thus, triazines cannot bind efficiently to the D1 protein and do not block photosynthetic electron transport (1, 2).

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to most soils; more readily adsorbed to muck (high OM) or clay soil than to soil of lower OM and clay content. Ametryn adsorbs more strongly to soil than do most commercially available triazines.

K_{oc} and K_d: Average K_{oc} is 300 mL/g (4); K_{oc} 205 mL/g and K_d 1.1 mL/g for a sand with 0.9% OM, 2.2% clay, and pH 6.5; K_{oc} 96 and K_d 1.1 mL/g for a sandy loam with 1.9% OM, 16.8% clay, and pH 7.5; K_{oc} 257 mL/g and K_d 1.2 mL/g for a loam with 0.8% OM, 9% clay, and pH 6.7; K_{oc} 927 mL/g and K_d 26.2 mL/g for a clay with 4.8% OM, 42% clay, and pH 5.9

Transformation:

Photodegradation: Half-life was 212 d in water at pH 7 with natural light and 5-29 C. The soil photolysis half-life was 108 d on a sandy loam at 5-29 C with natural light. Photodegradation is of minor importance in the field except where prolonged drought after application allows ametryn to remain on the soil surface.

Other degradation: Half-life was 37 d for aerobic metabolism in a sandy loam at 25 C, with *N*-deethylated ametryn [*N*-(1-methylethyl)-6-methylthio-1,3,5-triazine-2,4-diamine] as the major degradation product (11.9% of applied after 14 d), and about 39% of the applied mineralized to CO_2. Ametryn is stable for anaerobic metabolism in a sandy loam at 25 C, producing primarily *N*-deethylated ametryn (7.3% after 31 d). Biological degradation is of major importance in ametryn dissipation. Ametryn is not hydrolyzed non-biologically at pH 5, 7, and 9.

Persistence: Average field half-life is 60 d (4). The persistence of ametryn in soils across the continental U.S. compares closely with prometryn. In more tropical conditions (Hawaii and Puerto Rico), ametryn provides better weed control and its residual life in the soil often is extended to several mo.

Field experiments: Half-lives in bareground dissipation studies at 0-15 cm after applying in a single application the maximum rate per year: 11 d for a silt loam with 0.9% OM and pH 6.9 in Louisiana; 48 d for a sandy loam with 1.6% OM and pH 6.6 in Illinois; 88 d for a loam with 1.5% OM and pH 8.1 in Hawaii. Application rate, and edaphic and environmental conditions can greatly impact half-life.

Mobility: In field experiments conducted in corn grown in Illinois, and sugarcane in Louisiana, no quantifiable ametryn residues (LOD = 10 µg/kg) were found below 30 cm.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade ametryn unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1160 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat >5.17 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

EVIK 80W: Oral LD_{50} rat, 1950 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >2.5 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

21-d dermal, rabbit: NOEL 100 mg/kg/d; reduced body weight gain at 1000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 1.5 mg/kg/d; not carcinogenic; reduced body weight and reduced weight gain at 1000 and 2000 mg/kg

24-mo dietary, rat: NOEL 2.5 mg/kg/d; not carcinogenic; reduced body weight and reduced weight gain at ≥500 mg/kg; liver effects at 2000 mg/kg

12-mo dietary, dog: NOEL 10 mg/kg/d; liver and kidney effects at ≥2000 mg/kg

Teratogenicity:

Rat: NOEL 5 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 10 mg/kg/d, developmental 60 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL maternal 20 mg/kg, developmental 2000 mg/kg; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Chinese hamster/nucleus anomaly, negative

DNA damage/repair: Rat hepatocytes, negative; Human fibroblasts, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg, 8-d dietary LC_{50}, >20,000 mg/kg; Mallard duck oral LD_{50}, >4640 mg/kg, 8-d dietary LC_{50}, >10,000 mg/kg; Honey bee oral LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 45.9 mg/L; Bluegill sunfish 96-h LC_{50}, 4.1 mg/L; Goldfish 96-h LC_{50}, 14.1 mg/L; Rainbow trout 96-h LC_{50}, 8.8 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Synthesized by successive *N*-alkylations and thioalkylation of cyanuric chloride

Purification of technical: Extraction and crystallization from water/toluene

Analytical methods: Crop samples are extracted by reflux in 90% methanol. The extract is acidified and partitioned with hexane to remove co-extractives. Aqueous fraction is then made basic and residues are partitioned into dichloromethane. Extracts are analyzed by GC with flame photometric detection in the sulphur-selective mode. Soil samples are extracted with 80% acetonitrile, partitioned into dichloromethane, and analyzed by GC with N/P detection. Water samples are partitioned with dichloromethane, the organic phase is concentrated, and residues determined by GC with N/P or mass selective detection. In technical samples and formulated products, ametryn is determined by GC and polar impurities by HPLC.

Historical: Synthesis and testing of triazine compounds as herbicides began in 1952 in the Geigy laboratories in Basel, Switzerland. Ametryn was first released for experiment station evaluation in 1959 and became commercially available for use in sugarcane and pineapple in 1964. First reported in 1960 (3).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Ebert and Dumford. 1976. Res. Rev. 65:1.
2. Esser, H. O. et al. 1975. *In* Kearney, P. C. and D. D. Kaufman, eds., Herbicides: Chemistry, Degradation, and Mode of Action. Marcel Dekker, Inc., New York.
3. Gysin and Knusli. 1960. Adv. Pest Control Res. 3:289.
4. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

amicarbazone

CAS #: 129909-90-6 $5^{(C_1)}$

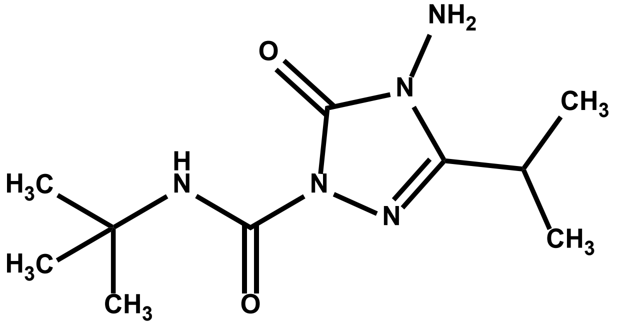
4-amino-*N*-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1*H*-1,2,4-triazole-1-carboxamide

NOMENCLATURE

Common name: amicarbazone (ISO 1750 accepted)
Other name(s): BAY MKH 3586; BAY 314666; 4-amino-*N*-*tert*-butyl-4,5-dihydro-3-isopropyl-5-oxo-1*H*-1,2,4-triazole-1-carboxamide
Trade name(s): NA
Chemical family: triazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
amicarbazone



Molecular formula: $C_{10}H_{19}N_5O_2$
Molecular weight: 241.29 g/mole
Description: Colorless crystals
Density: 1.12 g/mL
Melting point: 137.5 C
Boiling point: NA
Vapor pressure: 1.3×10^{-6} Pa (20 C); 3.0×10^{-6} Pa (25 C)
Solubility: water, 4600 mg/L (pH 4-9)
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 1.18 (pH 4); 1.23 (pH 7); 1.23 (pH 9)

HERBICIDAL USE

Amicarbazone has shown promise to control a broad spectrum of weeds including velvetleaf (*Abutilon theophrasti*), common lambsquarters (*Chenopodium album*), pigweed species (*Amaranthus spp.*), common cocklebur (*Xanthium strumarium*), and morningglory species (*Ipomoea spp*) among others at rates of 250 to 500 g/ha. In sugarcane, amicarbazone will control painted wild poinsettia (*Euphorbia heterophylla*), morningglories, southern sandbur (Cenchrus echinatus), and marmeladegrass (*Brachiaria plantaginea*) among others at 700 to 1200 g/ha.

USE PRECAUTIONS

Fire hazard: None known
Corrosiveness: None known
Storage stability: Stable when stored under normal conditions
Emergency exposure: Eyes: rinse immediately; skin: wash affected areas with soap and water
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Susceptible plants demonstrate chlorosis, stunted growth, tissue necrosis beginning at leaf edges and progressing across the leaf and stem tissue, and eventual death.
Absorption/translocation: Plant uptake occurs via the roots. Leaf absorption has also been demonstrated on weeds exhibiting acute contact activity, and this can be enhanced with the addition of an adjuvant.
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 23-37 mL/g on silt loam
Transformation:
Photodegradation: Stable in sterile water, pH 7; natural water, DT_{50} 66 d; soil DT_{50} 54 d
Other degradation: Aerobic, DT_{50} 50 d
Persistence:
Field experiments: Nebraska and Wisconsin, DT_{50} 18-24 d
Volatilization: Moderate

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, > 1015 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; inhalation LC_{50} (rat, 4-hr exposure), 2.242 mg/L
Subchronic toxicity:
90-d dietary, mouse: NA
Wildlife:
Avian toxicity: Oral LD_{50} bobwhite quail, >2000 mg/kg; dietary LC_{50} bobwhite quail, >5000 mg/kg
Aquatic toxicity: LC_{50} bluegill sunfish, >129 mg/L (96h); rainbow trout, >120 mg/L (96 h), Daphnia magna, >120 mg/L (48 h); EC_{50} Lemna gibba, 226 µg/L (48 h)
Others: Oral LD_{50} honeybee, 24.8 µg/bee; Contact LD_{50} honeybee, >200 µg/bee
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Philbrook, B.D., M. Kremer, K. H. Mueller, and R. Deege. 1999. BAY MKH 3586 – a new herbicide for broad spectrum weed control in corn (maize) and sugar cane. Proc. 1999 Br. Crop Prot. Conf. Vol. 1:29-34.

amidosulfuron

CAS #: 120923-37-7

$2^{(B)}$

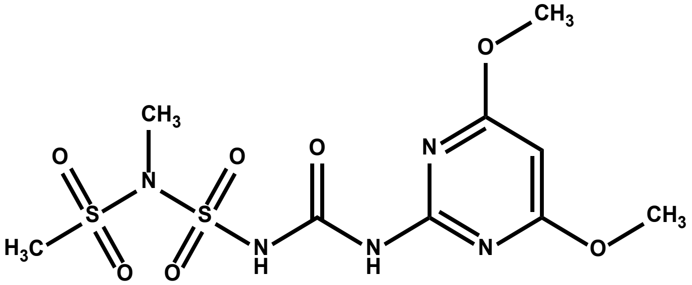
N-[[[[(4,6-dimethoxy-2-pyrimdinyl)amino]carbonyl]amino]
sulfonyl]-*N*-methylmethanesulfonamide

NOMENCLATURE

Common name: amidosulfuron (ISO approved)
Other name(s): AE F075032; HOE 075032; IUPAC
Trade name(s): ADRET; DRUID; GRATIL; CRODYL; HOESTAR; EAGLE; SQUIRE; TOSCA
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
amidosulfuron



Molecular formula: $C_9H_{15}N_5O_7S_2$
Molecular weight: 369.37 g/mole
Description: White, crystalline powder
Density: 1.5 g/mL
Melting point: 160-163 C
Boiling point: NA
Vapor pressure: 2.2 x 10^{-5} Pa (20 C)
Stability: Stable for 2 yrs at 25 C in unopened original containers
Solubility:
water, 3.3 mg/L (pH 3, 20 C); 9 mg/L (pH 5.8, 20 C); 13,500 mg/L (pH 10, 20 C)
pK_a: 3.58 (weak acid)
K_{ow}: log K_{ow} = 1.63 (pH 2, 20 C)

HERBICIDAL USE

Amidosulfuron is used for selective post-emergence broadleaf weed control in cereals, fields, and pastures. Use rates are 30-40 g a.i./ha. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: May give off toxic fumes if heated to decomposition
Corrosiveness: NA
Storage stability: Stable when stored at < (50 C)
Emergency exposure: Eyes: rinse immediately with running water for at least 15 mins. Skin: wash off affected area with soap and water.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Absorption/translocation: Absorbed by roots and leaves and translocated predominately by the phloem.
Symptomology: Chlorosis of meristem; typical symptoms of ALS-inhibiting herbicides
Metabolism in plants: The primary metabolite in tolerant crops and/or weeds is an O-demethylated metabolite of amidosulfuron.
Mechanism of resistance in weeds: Weeds that are resistant have a insensitive form of the ALS enzyme.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Other degradation: Hydrolysis occurs at pH 5, 7, and 9; DT$_{50}$ >500 at pH 7 and 9
Persistence:
Field: DT$_{50}$ of 44 d (loamy sand) to 63-231 d (clay soil at 85% field capacity at 10 C)
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade amidosulfuron unless otherwise indicated.
Acute toxicity:
Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rat, >4000 mg/kg, Inhalation LC$_{50}$, 50 mg/kg (4 h)
Chronic toxicity:
Rat 2-year feeding: NOEL 19.5 mg/kg/d
Teratogenicity: Non-teratogenic
Mutagenicity: Non-mutagenic
Wildlife:
Mallard duck LD$_{50}$, >2000 mg/kg; Bobwhite quail LD$_{50}$, >2000 mg/kg; rainbow trout LC$_{50}$ (96h), >320 mg/L; Water flea LC$_{50}$ (48h), 36-55 mg/L; Algae EC$_{50}$, 47 mg/L (72 h); Toxicity to honeybees, no

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: Product and residue analysis by HPLC (2)
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1. Roberts, T. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.
2. Barefoot, A.C. et al. 1995. Proc. British Crop Prot. Conf. Weeds. 2:707.

aminocyclopyrachlor

CAS #: 858956-08-8 $4^{(O)}$

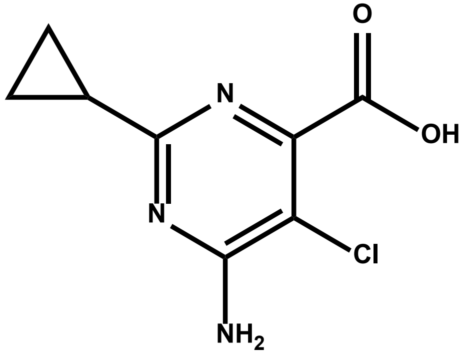
6-amino-5-chloro-2-cyclopropyl-4-pyrimidinecarboxylic acid

NOMENCLATURE

Common name: aminocyclopyrachlor (ANSI, BSI, ISO, WSSA)
Other name(s): DPX-MAT28 ; 6-amino-5-chloro-2-cyclopropylpyrimidine-4-carboxylic acid (IUPAC);
Trade name(s): PERSPECTIVE®, STREAMLINE®, VIEWPOINT®
Chemical family: pyridine carboxylic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *aminocyclopyrachlor*



Molecular formula: $C_8H_8ClN_3O_2$
Molecular weight: 213.62 g/mole
Description: Brown liquid
Density: 1.134 g/mL
Melting point: 140.5 C
Boiling point: 432.316°C at 760 mmHg
Vapor pressure: 4.89 $X10^{-8}$ kPa at 25 C
Stability: Stable under normal storage conditions
Solubility:
water 4.2 g/L (25 C)
organic solvents (25 C): NA
pK_a: 4.65
$logK_{ow}$: -1.12 pH 4;-2.48 pH 7

HERBICIDAL USE

Registered for use to control annual and perennial broadleaf weeds in uncultivated non-ag lands (e.g. airports, highways, railroad, etc.); uncultivated and non-producing agricultural land (e.g. fence row, barnyard, barrier strips, etc.); industrial sites; and natural areas (e.g. wildlife management areas, camp grounds, trails, etc.).

USE PRECAUTIONS

Fire hazard: Not a fire or explosion hazard.
Corrosiveness: Non-corrosive to spray equipment.
Storage stability: Stable at normal temperatures and storage conditions.
Cleaning glassware/spray equipment: NA
Emergency exposure:
Eyes: Hold eye open and rinse slowly and gently with water for 15-20 minutes. Remove contact lenses, if present, after the first 5 minutes, then continue rinsing eye.
For skin or clothing: Take off contaminated clothing. Rinse skin immediately with plenty of water for 15-20 minutes. Call a poison control center or doctor for further treatment advice.
Incompatibilities: Compatible with most other pesticides and liquid fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Aminocyclopyrachlor is a systemic, ambi-mobile growth-regulator herbicide. (For more details see page 12).
Symptomology: As the compound translocates and accumulates in meristematic tissue it causes uneven cell division and growth resulting in death of susceptible plant species. Aminopyralid provides a broad spectrum of broadleaf weed control. Within hours or days of application, aminopyralid causes symptoms such as thickened, curved and twisted stems and leaves, cupping and crinkling of leaves, stem cracking, narrow leaves with callus tissue, hardened growth on stems, enlarged roots and proliferated growth. Most susceptible annual plants are controlled within 4 to 8 weeks after application. Control of perennial herbaceous broadleaf plants or woody plants may take 2 months or more after application.
Absorption: Readily absorbed through leaves, green stems or roots.
Translocation: Transported in both phloem and xylem, accumulating in meristematic and other metabolically active tissues
Metabolism in plants:
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:
$K_{oc:}$: 26 in a Drummer clay loam (pH 6.4, %OM 5.7), 5.2 in a California loam (pH 8.73, %OM 0.8), 2.0 in a Nambsheim sandy loam (pH 8.09, %OM 1.4), 3.2 in a Lleida silty clay (pH 7.83, %OM 2.6), and 22 in a Sassafras sandy loam (pH 5.67, %OM 1.8).
Transformation:
Photodegradation: Negligible losses
Other degradation: Aminocyclopyrachlor acid had a linear half-life of 433.2 days in a sandy loam soil (pH 8.09, %OM 2.2), 113.6 days in a silty clay loam (pH 6.45, %OM not available), and 126 days in a clay loam soil (pH 6.4, %OM 6.5). Observed half-lives were >120 days, >110 days and >110 days, respectively. No major transformation products were found.
Persistence: Aminocyclopyrachlor slowly degrades by aerobic microbial metabolism with half-lives, ranging from 114-433 days in different soils. It is stable to degradation

via other pathways..
Mobility: Aminocyclopyrachlor is expected to be highly mobile in the environment.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade aaminocyclopyrachlor unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat >5000 mg/kg;
Subchronic toxicity:
90-d dietary, mouse: NOEL >1424 mg/kg/d;
90-d dietary, dog: NOAEL >426 mg/kg/d
21-d dermal, rat: NOEL 1000 mg/kg/d
Chronic toxicity:
95-d dietary, mouse: Systemic NOEL = 7000 ppm (1088 mg/kg/day (males) and 1623 mg/kg/day (females)).
24-mo dietary, rat: Study 1, NOEL 500 mg/kg; MTD was exceeded at 5000 mg/kg; reduced body weight and food consumption, and liver necrosis at 5000 mg/kg; liver and thyroid tumors at doses above the MTD; nasal tumors at levels below the MTD, In study 2, NOEL 200 mg/kg; reduced body weight and increased nasal tumors at 1000 mg/kg
Teratogenicity:
Rat: The NOAEL is 17,000 ppm (equivalent to 1285/1454 mg/kg in males/females).not teratogenic
Rabbit: The developmental NOAEL is 1000 mg/kg/day; not teratogenic
Reproduction:
Rat: The developmental NOAEL is 1000 mg/kg/day
Mutagenicity:
Gene mutation: negative
Structural chromosome aberration: negative
DNA damage/repair: negative
Wildlife:
Bobwhite quail oral LD_{50}, >2075 mg/kg bw; 8-dietary LC_{50}, >5290 mg/kg; Mallard duck 8-d dietary LC_{50}, >5290 mg/kg;; Daphnia 48-h LC_{50}, >19.9 mg/L; Bluegill sunfish >120 mg/L - Rainbow trout LC_{50}, > 13 mg/L
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): DuPont Crop Protection
Reference(s):

1. National Library of Medicine HSDB Database: http://toxnet.nlm.nih.gov/cgi-bin/sis/search/a?dbs+hsdb:@term+@DOCNO+7981. Accessed 16 January, 2014.

aminopyralid

4-amino-3,6-dichloro-2-pyridinecarboxylic acid

CAS # 150114-71-9. **4$^{(O)}$**

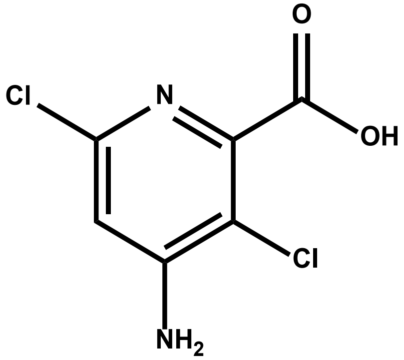
NOMENCLATURE

Common name: aminopyralid (ISO approved)
Other name(s): DE-750; 4-amino-3,6-dichloropyridine-2-carboxylic acid (IUPAC)
Trade name(s): AMINOPYRALID TECHNICAL, CLEANWAVE, MILESTONE, FOREFRONT R&P, CAPSTONE, MILESTONE VM PLUS, PASTURALL, GRAZONNEXT, CHAPARREL, GRAZONNEXT HL, PASTURALL HL, FOREFRONT HL, OPENSIGHT, OPENSIGHT WG
Chemical family: pyridine; picolinic acid; pyridinecarboxylic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure(s):

Aminopyralid acid



Molecular formula: *Acid* $C_6H_4Cl_2NO_2$;
Molecular weight: *Acid* 207.03 g/mole; *Potassium* salt 245.11 g/mole, TIPA salt 398.28 g/mole
Description: Off-white odorless powder
Density: 1.72 g/mL (20 C)
Melting point: 163.5 C
Boiling point: Decomposes upon melting
Vapor pressure: 9.52×10^{-9} Pa (20 C); 2.56×10^{-8} Pa (25 C)
Stability: Hydrolytically stable
Water solubility

pH 5	212 g/L
pH 7	205 g/L
pH 9	203 g/L
Unbuffered2	.48 g/L

Vapor Pressure 7.14×10^{-11} mm Hg
pKa 2.56

Log K_{ow}

Unbuffered	0.201
pH 5	-1.75
pH 7	-2.87
pH 9	-2.96

Organic Solvent Solubilities

Acetone	30 g/L
Ethyl Acetate	4 g/L
Methanol	50 g/L
1,2-dichloroethane	2 g/L
Xylene	43 mg/L
Heptane	less than 10 mg/L

HERBICIDAL USE

Aminopyralid is intended for use in rangeland, permanent grass pastures (including grasses grown for hay), Conservation Reserve Program (CRP) acres, non-cropland areas including airports, barrow ditches, communication transmission lines, electric power and utility rights-of-way, fencerows, gravel pits, industrial sites, military sites, mining and drilling areas, oil and gas pads, non-irrigation ditch banks, parking lots, petroleum tank farms, pipelines, roadsides, railroads, storage areas, storm water retention areas, substations, unimproved rough turf grasses, vacant lots and other non-crop residential areas; and natural areas (open space) for example, campgrounds, trailheads and trails, recreation areas, wildlife openings, and wildlife habitat and management areas, and including grazed areas in and around these sites as well as wheat (including spring wheat, winter wheat, and durum), oil palm and rubber plantations. It is permissible to treat non-irrigation ditch banks, seasonally dry wetlands (such as flood plains, deltas, marshes, swamps, or bogs) and transitional areas between upland and lowland sites. Aminopyralid can be used to the water's edge in riparian areas. Aminopyralid applied at 5 to 120 g ae/ha provides post emergence control of many broadleaf and some semi-woody weeds, including difficult to control invasive and noxious broadleaf weeds such as the biennial thistles (musk, bull and plumeless), Canada thistle, medusahead, musk thistle, Russian knapweed, spotted knapweed, squarrose knapweed, diffuse knapweed, and yellow starthistle. Depending on rate applied and weed species, aminopyralid can also provide residual or preemergence control of some germinating weed seeds and emerging seedlings. Aminopyralid is selective to grasses at typical use rates and most annual and perennial grasses are not adversely affected by post emergence applications in field situations. Aminopyralid is also available in premix formulations with 2, 4-D, fluroxypyr, triclopyr, and metsulfuron-methyl. In these premixes, aminopyralid contributes to control of a broad spectrum of broadleaf weeds and woody plants, including species in the genera *Eupatorium*, *Sida, Solidago*, *Symphoricarpos*, *Urtica*, *Vervain*, *Daucus and Vernonia.*
Use classification: General use

USE PRECAUTIONS

Fire hazard: Flash point not applicable (water-based material)
Corrosiveness: Not corrosive
Storage stability: Stable under normal conditions
Cleaning glassware/spray equipment: Rinse and flush equipment at least three times with water; add household ammonia at 1% v/v during the second rinse.

Emergency exposure: If in eyes: Hold eye open and rinse slowly and gently with water for 15-20 minutes. Remove contact lenses, if present, after the first 5 minutes and then continue rinsing. Call a poison control center or doctor for treatment advice.
Incompatibilities: All formulated products are compatible with most types of hard water.
Eye Contact: May cause eye irritation and slight corneal injury.
Skin Contact: Brief contact is essentially nonirritating to skin.
Skin Absorption: Prolonged skin contact is unlikely to result in absorption of harmful amounts.
Inhalation: No adverse effects are anticipated from single exposure to dust.
Ingestion: Very low toxicity if swallowed. Harmful effects not anticipated from swallowing small amounts.

BEHAVIOR IN PLANTS

Mechanism of action: Aminopyralid is a systemic, ambimobile growth-regulator herbicide. (more detaills on page 12.)
Symptomology: As the compound translocates and accumulates in meristematic tissue it causes uneven cell division and growth resulting in death of susceptible plant species. Aminopyralid provides a broad spectrum of broadleaf weed control. Within hours or days of application, aminopyralid causes symptoms such as thickened, curved and twisted stems and leaves, cupping and crinkling of leaves, stem cracking, narrow leaves with callus tissue, hardened growth on stems, enlarged roots and proliferated growth. Most susceptible annual plants are controlled within 4 to 8 weeks after application. Control of perennial herbaceous broadleaf plants or woody plants may take 2 months or more after application.
Absorption: Readily absorbed through leaves, green stems or roots.
Translocation: Transported in both phloem and xylem, accumulating in meristematic and other metabolically active tissues
Metabolism in plants: Detoxified through glucose conjugation followed by incorporation into cell wall constituents. The mechanism of grass crop tolerance is not solely the result of plant metabolism, rather it is likely that grass tolerance is result of the inability of the herbicides to effectively bind to protein receptor sites where they would otherwise bind and exert an herbicidal effect.
Non-herbicidal biological properties: None known.
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed.
K_d: 0.03 – 0.72 mL/g **K_{oc}:** Average 10.8 mL/g
Aminopyralid is dissociated and negatively charged in soil because of its low pKa and therefore can show some soil mobility. However, any potential for aminopyralid downward movement is substantially mitigated by the herbicide's low use rates.

Transformation:
Photodegradation: Aminopyralid's aqueous photolysis half-life is 0.6 d under standard conditions indicating rapid degradation in surface water. As a result of pyridine ring cleavage, aqueous photolysis degradation products are limited to small organic acids such as oxamic and malonamic acid which undergo further rapid degradation to CO_2. Aminopyralid is stable to hydrolysis and degrades very slowly under anaerobic conditions in aquatic sediments. Aminopyralid photolyzed moderately slowly on soil surfaces with a half-life of approximately 72 days, no degradates are produced by soil photolysis except for CO_2, non-extractable residues and small amounts of acidic organic volatiles.
Soil degradation: Aerobic microbial degradation is the primary means by which aminopyralid is degraded in soil. Only non-phytotoxic small organic acids are produced under aerobic soil conditions and these are rapidly metabolized further to CO_2. Under anaerobic conditions, such as occur in flooded soils, microbial degradation is slow and is not a significant route of degradation.
Animal metabolism: Aminopyralid does not breakdown upon ingestion by mammals and is excreted in urine and feces within 3 days of ingestion. Consequently, manure and slurry from animals fed aminopyralid-treated grass, hay or silage can contain aminopyralid residues that may be phytotoxic to susceptible plants. This slurry or manure should be applied to crops as specified on product labels and managed according to label precautions and restrictions.
Degradation in compost: Aminopyralid residue concentrations are not reduced in plant materials or manure during the thermophilic or curing phases of the composting process. Although degradation of residues does occur, plant biomass dry matter decline occurs at about the same rate or faster so aminopyralid concentrations are not altered or can increase slightly, as the compost dries, during compost preparation.
Persistence in soil: The rate of aminopyralid degradation in laboratory studies was somewhat variable in regulatory studies, with first-order half-lives ranging from 14 to 143 days in eight soil types with a mean value of 76 days. Under field conditions, degradation was much faster and less variable, with half-lives ranging from 6 to 74 days at 8 North American locations; the median North American soil half-life was 32 days. This data set included two United States sites (California and Mississippi) where the soil half-life averaged about 28 days (range 25 to 32 days) with minimal leaching below the 15 to 30 cm (6 to 12 inches) horizon depth. No metabolites of concern were produced in any environmental matrix.
Mobility in soil: Laboratory experiments yielded an average K_{oc} of 10.8 L/kg, indicating some potential for mobility. However, under actual use conditions, aminopyralid becomes more tightly bound to the soil particles with time, so mobility is further reduced with time after application and field experiments show very limited movement in the soil profile. Experiments were conducted to compare the soil adsorption of aminopyralid to that of picloram and clopyralid. Aminopyralid bound

more tightly than clopyralid to six of the eight soils tested and soil sorption of aminopyralid was greater than that of picloram.

Volatilization: Extremely low potential for volatility loss due to low vapor pressure

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade aminopyralid acid unless otherwise indicated.

Acute toxicity:

Ingestion: LD50, Rat, male and female > 5,000 mg/kg

Skin Absorption: LD50, Rat, male and female >5,000 mg/kg

Inhalation: LC50, 4 h, Aerosol, Rat, male and female >5.5 mg/l

Sensitization Skin: Did not cause allergic skin reactions when tested in guinea pigs.

The overall toxicological profile of aminopyralid is very favorable. It is not acutely toxic, does not pose an inhalation hazard, nor is it a skin sensitizer. No evidence of mutagenic or carcinogenic potential was obtained from any study. Aminopyralid showed no teratogenic effects in either rats or rabbits.

Repeated Dose Toxicity: Aminopyralid is practically non-toxic to mammals (rats, mice, rabbits, and dogs) based on an oral LD_{50} > 5,000 mg kg-1. In a metabolism study in rats, aminopyralid was excreted unchanged, indicating an absence of metabolism. Repeated administration of aminopyralid was not associated with bioaccumulation in tissues. In animals, the most sensitive effect and target organ was enlargement of the rat cecum, a component of the rat gastrointestinal tract, likely due to physical irritation.

Chronic Toxicity and Carcinogenicity:

Carcinogenicity: Did not cause cancer in laboratory animals and has been classified by US EPA as "not likely" to be carcinogenic to humans. There were no increases in tumors in any studies.

Developmental Toxicity: Did not cause birth defects or other effects in the fetus even at doses which caused toxic effects in the mother.

Reproductive Toxicity: In animal studies, did not interfere with reproduction. Tests indicate that aminopyralid is not a reproductive hazard or concern.

Genetic Toxicology: In vitro genetic toxicity studies were predominantly negative. Animal genetic toxicity studies were negative.

Chronic Exposure: EPA has concluded that chronic exposure to aminopyralid from food and water will utilize <1% of the chronic Population Adjusted Dose (cPAD, also called the "aggregate exposure Risk Cup") for the general U.S. population and all population subgroups. Regulatory concern is not justified until the cPAD exceeds 100%.

Avian Acute and Subacute Toxicity: The acute oral and dietary toxicity of aminopyralid to birds can be categorized as practically non-toxic. Bobwhite quail acute oral LD50 > 2250 mg ae/kg bw, bobwhite quail acute dietary LC50 > 5620 mg ae/kg diet, mallard duck acute dietary LC50 > 5620 mg ae/kg diet .

Avian Reproductive Toxicity: There were no treatment-related effects of aminopyralid on reproductive parameters in bobwhite quail and mallard duck at all dietary concentrations up to and including the highest concentration tested of 2700 mg ae/kg diet: Long-term reproductive NOEC, 2700 mg/kg; Mallard duck oral LD_{50}, 5620 mg/kg; Long-term reproductive NOEC, 2700 mg/kg;

Fish and Amphibian Acute and Chronic Toxicity: The acute and chronic toxicity of aminopyralid to fish can be categorized as practically non-toxic. Rainbow trout 96 hr LC50 > 100 mg ae/L, bluegill perch 96 hr LC50 > 100 mg ae/L, sheepshead minnow 96 hr LC50 > 100 mg ae/L, fathead minnow early life stage NOEC = 1.36 mg ae/L, Larval Northern leopard frog 96 hr LC50 > 100 mg ae/L

Aquatic Invertebrate Toxicity: The acute and chronic toxicity to most aquatic invertebrates can be categorized as practically non-toxic; aminopyralid is classified as slightly toxic to the eastern oyster although there was no effect at the highest concentration tested (89 mg/L). Daphnia magna acute toxicity 48 hr EC50 > 100 mg ae/L, mysid shrimp acute toxicity 96 hr LC50 > 100 mg ae/L, Eastern oyster acute toxicity 48 hr EC50 > 89 mg ae/L, Daphnid growth and reproduction NOEC = 100 mg ae/L, Freshwater Sediment Dweller (Chironomus riparius) 28-Day Lifecycle Water Exposure EC50 = 680-mg ae/L and NOEC = 130 mg ae/l,

Aquatic Plant Toxicity: Duckweed 14-d EC50 = >88 mg ae/L, Freshwater green alga 96-hr EC50 = 32 mg ae/L, Saltwater diatom 120-hr EC50 > 100 mg ae/L, Freshwater diatom 96-hr EC50 = 14 mg ae/L, Blue green alga 120-hr EC50 = 27 mg ae/L

Honeybee Acute Contact and Other Terrestrial Invertebrate Toxicity: Aminopyralid was non-toxic to honeybees and earthworms in acute toxicity studies. Acute Honeybee Contact Toxicity 48 hr LD50> 100 µg ae/bee, Acute Honeybee Oral Toxicity 48 hr LD50> 120 µg ae/bee, Earthworm 14-Day Acute Toxicity LC50> 1000 mg ae/kg/soil.

SYNTHESIS AND ANALYTICAL METHODS

The aminopyralid Enforcement Analytical Method is a reverse phase isocratic liquid chromatographic separation with UV detection at 270 nm. Determination of the weight percent of the active ingredient and impurities present is performed by internal standard calibration. Residue analysis of aminopyralid in water, soil, crop, and tissue samples is done by LC-MS/MS with limits of detection as low as 1 µg/L or µg/kg.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Dow AgroSciences

References:

1. Almquist T.L. and R. G. Lym. 2010. Invasive Plant Science and Management 3:155–168.
2. Bukun B., D.L. Shaner, S. Nissen, P. Westra and G. Brunk. 2010. *Weed Science.* 58, 473-477.
3. Enloe, S.F., G.B. Kyser, S.A. Dewey, V.F. Peterson and J.M. DiTomaso. 2008. Invasive Plant Science and Management 1(4):385–389.
4. Enloe, S.F., R.G Lym, R Wilson, P Westra, S.J. Nissen, G Beck, M. Moechnig, V.F. Peterson, , R.A Masters and M. B. Halstvedt. 2007. Weed Technology 21:890–894.
5. Fast BJ, Ferrell JA, Macdonald GE, Krutz LJ, WN Kline.

2010. *Weed Science.* 58, 484-489.

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7. Kyser, G.B., V.F. Peterson, J.S. Davy and J.M. DiTomaso. 2012. Rangeland Ecol Manage 65:418–425.
8. Mikkelson J.R. and R.G. Lym. 2013. Invasive Plant Science and Management 6:30-35
9. Syracuse Environmental Research Associates, Inc. 2007. Aminopyralid Human health and ecological risk assessment - Final Report. SERA TR 052-04-04a. Report dated June 28, 2007. Available at: http://www.fs.fed.us/foresthealth/pesticide/risk.shtml

amitrole

1*H*-1,2,4-triazol-3-amine

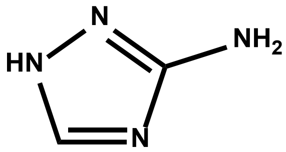
CAS #: 61-82-5 $11^{(F_3)}$

NOMENCLATURE

Common name: amitrole (ANSI, BSI, ISO, WSSA)
Other name(s): aminotriazole; 1*H*-1,2,4-triazol-3-amine (IUPAC); 3-amino-s-triazole; 3-amino-1*H*-1,2,4-triazole; 3-amino-1,2,4-triazole
Trade name(s): AMITROL-T™; AMIZOL®; LIQUID AMIZINE®; AMEROLE; ATA; AT 90; AZOLE; HERBIZOLE; VOPOX; GRANULAT 371; WEEDAZIN; WEEDAZOL
Chemical family: triazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:



Molecular formula: $C_2H_4N_4$
Molecular weight: 84.08 g/mole
Description: Off-white crystalline powder, odorless when pure
Density: 1.14 g/mL (20 C)
Melting point: 159 C
Boiling point: NA
Vapor pressure: 5.86×10^{-5} Pa (20 – 25 C)
Stability: NA
Solubility:
water 280,000 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone insoluble ethanol 260 (75 C)
diesel oil insoluble
ethyl acetate sparingly soluble
ether insoluble kerosene insoluble
pK_a: 9.83 (weak base) (17)
K_{ow}: NA
Other properties: Forms salts with most acids or bases; a powerful chelating agent.

HERBICIDAL USE

Amitrole can be applied broadcast postemergence to weed foliage at 2-9 kg ai/ha in non-crop areas such as railroad rights-of-way, roadsides, fence rows, and utility installations, or POST-directed at 2-9 kg/ha in hardwood nurseries. It also can be applied on these sites using 1.2-4.8 g? ai/L in a spray-to-wet application. Amitrole controls many annual and perennial grass and broadleaf weeds.

USE PRECAUTIONS

Fire hazard: AMITROLE-T (aqueous) and AMIZOL (dry powder) are non-flammable.
Corrosiveness: Mildly corrosive to iron, aluminum, copper, and copper alloys.
Storage stability: No shelf life limitations
Cleaning glassware/spray equipment: Wash with water.
Emergency exposure: Thiocyanate poisoning may occur when AMITROL-T is ingested. Do not induce vomiting. Rinse mouth and drink 2-3 cups of water and seek medical advice.
Incompatibilities: Suitable for use with hard water. Not intended for mixing with other pesticides and fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits accumulation of chlorophyll and carotenoids in the light (1), although the specific site of action has not been determined. Precursors of carotenoid synthesis, including phytoene, phytofluene, carotenes, and lycopene accumulate in amintrole-treated plants (2), suggesting that phytoene desaturase, lycopene cyclase, imidazolegycerol phosphate dehydrase, nitrate reductase, or catalase may be inhibited. Other research (8), however, indicates that the histidine, carotenoid, and chlorophyll biosynthetic pathways probably are not the primary sites of amitrole action. Instead, amitrole may have a greater effect on cell division and elongation than on pigment biosynthesis. (For more detail see page 13.)
Symptomology: The primary symptom is bleaching (albinism) in leaves and shoots, and is most evident in meristems and developing leaves. Bleached tissues eventually wilt and become necrotic.
Absorption: Amitrole absorption into roots or penetration across the leaf cuticle is extremely rapid. Over 90% of foliar-applied amitrole penetrated the shoot of field horsetail 1 d after application (7). Foliar uptake rate of amitrole is considerably faster than certain otherpostemergence herbicides, including glyphosate, asulam, and fosamine (7, 14). However, amitrole may be partially bound to cuticular wax during initial uptake stages. Transport of amitrole across the plasma membrane is probably a passive process, occurring by simple diffusion (12).
Translocation: Amitrole is polar and nonionized, and is strongly mobile in the apoplast (including the xylem), and is largely retained in the phloem once it has crossed the plasma membrane (4). Consequently, amitrole is considered ambimobile, translocating in both apoplasm and symplasm. Based on the injury pattern, the herbicide appears to accumulate at the growing points.
Metabolism in plants: Amitrole metabolizes only slowly in field horsetail (15). The proportion of parent amitrole in shoot extracts after 1 and 8 wk was 76 and 81%, respectively. The primary metabolite (6-10%) was a serine conjugate forming ®-(3-amino-1,2,4-triazol-1-yl)-〈-alanine. Amitrole may also conjugate with glycine (6) in some plants, and may complex with tannins. Differential susceptibility to amitrole has been associated with varying rates of herbicide metabolism.

Non-herbicidal biological properties: Amitrole appears to have insecticidal effects on *Protophormia terraenovae* larvae (16). The toxicity was due to peroxidase inhibition and consequent disruption of cuticle hardening.

Mechanism of resistance in weeds: A biotype of rigid ryegrass from Australia is resistant to amitrole (5). The proposed mechanism of resistance is enhanced metabolism or sequestration of the herbicide within the leaf. In addition, Arabidopsis and tobacco lines have been selected for amitrole resistance.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 100 mL/g (17)

Transformation:

Photodegradation: Minor losses

Other degradation: NA

Persistence: Average field half-life is 14 d (17)

Mobility: NA

Volatilization: Minor losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade amitrole unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, >5000 mg/kg, male mouse, >5000 mg/kg; Dernal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

Subchronic toxicity: NA

Chronic toxicity:

16-mo dietary, rat: NOEL NA; enlarged thyroid after 90 d at 50 mg/kg/d in males; rats fed 500 mg/kg/d for 120 d and then returned to an amitrole-free diet 14 d before sacrifice, appeared to have normal thyroids.

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Mallard duck LD_{50}, 2000 mg/kg.

Use classification: Restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Condensation of formic acid with aminoguanidine

Purification of technical: Repeated recrystallizations from methanol

Analytical methods: Residues in sugarcane can be determined with a sensitivity of 0.1 µg (10). Analysis of formulated products by GC with flame ionization detection (11), by acid-base titration, or by formation of a silver complex during titration with silver salts; resides in soils determined by colorimetry (9, 13)

Historical: First reported in 1953 (3); introduced in 1954 by Union Carbide, U.S. patent 2,670,282

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Dow AgroSciences

Reference(s):

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2. Barry and Pallett. 1990. Z. Naturforsch. 45c:492.
3. Behrens, R. 1953. Proc. North Cent. Weed Control Conf. p. 61.
4. Bromilow, R.H. et al. 1990. Pestic. Sci. 30:1.
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11. Jacques, A. 1984. Anal. Methods Pestic. Plant Growth Regul. 13:191.
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13. Løkke, H. 1980. J. Chromatogr. 20:234.
14. Marshall, G. et al. 1987. Pestic. Sci. 18:55.
15. Marshall, G. et al. 1987. Pestic. Sci. 18:65.
16. Messner, B. 1987. Archiv. Phytopathol. Pflanzensch. 23:153.
17. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

AMS

CAS #: 7773-06-0 **NC**

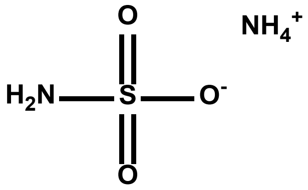
monoammonium sulfamate

NOMENCLATURE

Common name: AMS (WSSA)
Other name(s): ammonium sulphamate (ISO); ammonium sulfamidate (IUPAC)
Trade name(s): AMMATE® X-NI; AMICIDE; IKURIN
Chemical family: None generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
AMS



$H_2N-S(=O)_2-O^- \quad NH_4^+$

Molecular formula: $H_6N_2O_3S$
Molecular weight: 114.12 g/mole
Description: Crystalline solid, odorless
Density: NA
Melting point: 131-132 C
Boiling point: NA
Vapor pressure: Negligible
Stability: Decomposes at 160 C; stable to UV light
Solubility:
water 2,160,000 mg/L (25 C)
organic solvents (25 C):
soluble in formamide, glycerol, and glycols
pK_a: 0.9 (1)
K_{ow}: NA

HERBICIDAL USE

AMS can be applied POST at 64 kg ai/ha in 935 L ai?/ha of water to control actively growing brush species such as oaks, maples, ash spp., pines, and spruces.

USE PRECAUTIONS

Fire hazard: AMS has fire retardant properties
Corrosiveness: AMMATE is corrosive. Use of AMMATE as an oil-water emulsion minimizes corrosion of equipment. An asphaltic base paint protects equipment, as does coating equipment surfaces with oil when not in use.
Storage stability: Stable under normal storage conditions. Crystals are hygroscopic; keep containers tightly closed.
Cleaning glassware/spray equipment: Wash with water.
Emergency exposure: Wash skin with water
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: NA
Symptomology: NA
Absorption/translocation: Rapidly absorbed by foliage and green stems. Spreader-stickers or application in oil-water emulsion improves wetting. Crystals or concentrated solutions applied to freshly cut woody stems are readily absorbed. AMS translocates in woody and in herbaceous plants (2, 4).
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Probably weakly adsorbed by soil, based on a lack of response to different soil characteristics and its behavior in field plots (3)
K_{oc}: Average is 30 mL/g (estimated) (1)
Transformation:
Photodegradation: Does not photodegrade
Other degradation: Strains of *Aureobasidum (Pullularia) pullulans, Aphalosporium acremonium*, and two unidentified species of *Achromobacter* and *Flavobacterium* used Na sulfamate as a source of nitrogen. Both the fungi and bacteria converted sulfamate to sulfate in approximately equimolar proportions to the amount of nitrogen assimilated (6).
Persistence: Average field half-life is 14 d (1); under humid eastern U.S. conditions, weed control efficacy of 1.47 kg AMS per 100 m^2 disappears after 6-8 wk (5)
Mobility: Leaches readily like chlorate, based on a lack of response to soil characteristics and its behavior in field plots (3)
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade AMS unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 3900 mg/kg; Dermal LD_{50}, NA; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation, NA
Subchronic toxicity: NA
Chronic toxicity:
105-d dietary rat: NOEL NA; no effects at 10,000 mg/L; growth inhibition, but no histological effects at 20,000 mg/L
Teratogenicity: NA
Reproduction:
Rat: NOEL NA; reproduction not impaired at 17.5 or 25 mg/kg/d for 15 mo
Mutagenicity:
Gene mutation: Ames test, negative
Wildlife:AMS technical: Bobwhite quail oral LD_{50}, 3000 mg/kg
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Neutralization of NH_4OH with sulfamic acid (prepared by reacting urea and oleum).

Purification of technical: Purified AMS is available as a laboratory reagent.

Analytical methods: AMS residues can be determined in certain fruits by measuring absorption at 665 nm.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

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2. Carvell, K. L. 1955. Forest Sci. 1:41.
3. Crafts, A. S. 1945. Hilgardia 16:483.
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5. DeFrance, J. A. 1943. Proc. Am. Soc. Hort. Sci. 43:336.
6. Jensen, H. L. 1963. J. Appl. Bacteriol. 26:253.

anilofos

CAS #: 64249-01-0 $15^{(K_3)}$

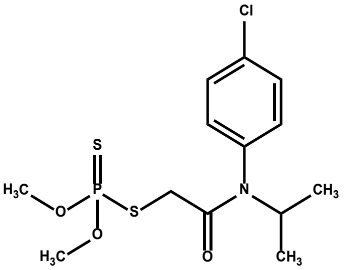
S-[2-[(4-chlorophenyl)(1-methylethyl)amino]-2-oxoethyl]
O,*O*-dimethyl phosphorodithioate

NOMENCLATURE

Common name: anilofos (ISO 1750 published)
Other name(s): *S*-4-chloro-*N*-isopropylcarbaniloylmethyl *O*,*O*-dimethyl phosphorodithioate (IUPAC)
Trade name(s): ANILOGUARD®; NIDAN
Chemical family: acetamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *anilofos*



Molecular formula: $C_{13}H_{19}ClNO_3PS_2$
Molecular weight: 367.85 g/mole
Description: Yellow liquid
Density: 11.27 g/mole
Melting point: 167 C
Boiling point: 50.5 – 52.5 C
(comment: boiling point is lower than melting point? Measured at different pressures?))
Vapor pressure: 2.2 x 10^{-3} (60 C)
Stability: Stable at pH 5-9 (22 C)
Solubility:
  water 13.6 mg/L (20 C)
  toluene > 1000 g/L
  ethyl acetate > 200 g/L hexane 12 g/L (25 C)
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 3.81 (25 C)

HERBICIDAL USE

Anilofos is a preemergence and early postemergence herbicide used for the control of annual grasses, sedges and selected broadleaved weeds in transplanted and direct seeded rice at the rate of 300-450 g/ha.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: Brass and copper can be corroded.
Storage stability: May undergo violent decomposition above 130 C.
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: Alkaline materials can cause hydrolysis.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits cell division and cell elongation.
Symptomology: Shoot and root growth is inhibited.
Absorption/translocation: Absorbed through roots and to some extent, through the leaves.
Metabolism in plants: NA
Non-herbicidal biological properties: None known.
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation*:* Typical degradation for a phosphoric acid compound, with chloroaniline and CO_2 as end products.
Persistence: Field dissipation DT_{50} = 30-45 d
Mobility: NA
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade anilofos unless otherwise indicated.
  Acute toxicity: Oral LD_{50} rat, >830 mg/kg; Dermal rabbit LD_{50}, >2000 mg/kg; 26-h inhalation LC_{50} rat, 26 mg/L.
Mutagenicity: Non-mutagenic.
Wildlife:
  Japanese quail oral LD_{50}, 3360 mg/kg; LC_{50} rainbow trout, 2.8 mg/L; (96 h); EC_{50} Daphnia magna, > 56 mg/L (48 h).
Use classification: General use.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Gharda.

asulam

methyl [(4-aminophenyl)sulfonyl]carbamate

CAS # Acid: 3337-71-1
Na salt: 2302-17-2

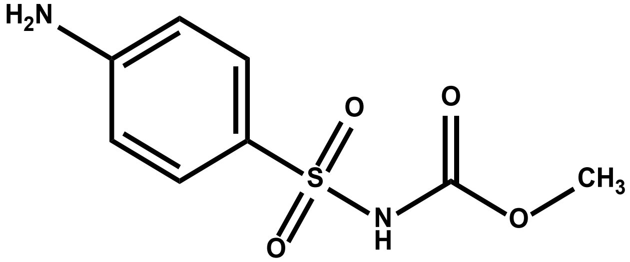
18$^{(I)}$

NOMENCLATURE

Common name: asulam (ANSI, BSI, ISO, WSSA)
Other name(s): asulam sodium; asulame; F-150; M&B 9057; methyl sulfanilycarbamate (IUPAC); methyl 4-aminobenzenesulphonylcarbamate; methyl 4-aminophenysulphonylcarbamate.
Trade name(s): ASILAN®; ASULOX®; JONNIX
Chemical family: carbamate; organophosphorus; sulfonamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *asulam acid*



Molecular formula: *Acid* $C_8H_{10}N_2O_4S$; *Na salt* $C_8H_9N_2NaO_4S$; *K salt* $C_8H_9KN_2O_4S$
Molecular weight: *Acid* 230.24 g/mole; *Na salt* 252.22 g/mole; *K salt* 268.33 g/mole
Description: Pale cream to buff crystals, faint characteristics odor
Density: 0.5 g/mL (packed)
Melting point: 135-137 C with decomposition
Boiling point: NA
Vapor pressure: 1.3 x 10^{-5} Pa (25 C)
Stability: Hydrolyzes in acid solution; stable in alkaline solution (maximum stability at pH 10)
Solubility:
water 534,000 mg/L (27 C)
organic solvents g/100 mL (25 C)
acetone 30
dichloromethane 0.31
ethanol moderately soluble
n-hexane 0.0013
hydrocarbon >2
methanol 2.3
pK_a: 4.82 (weak acid)
K_{ow}: 1.01

HERBICIDAL USE

Asulam is applied as follows: POST at 1.12-4 kg ae/ha in sugarcane for control of many grass weed including johnsongrass, and in pastures and forest sites for control of *Rumex spp*. and *Pteridium aquilinum*; POST at 0.8-1.6 kg ae/ha in alfalfa, flax, and chicory; POST at 3 kg ae/ha in poppies. Asulam controls many annual and perennial broadleaf and grass weeds, as well as some perennial ferns.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: NA
Storage stability: Stable for >2 yr under normal conditions
Cleaning glassware/spray equipment: Wash with detergent and water
Incompatibilities: Usually compatible with most materials

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Asulam appears to inhibit cell division and expansion in plant meristems, perhaps by interfering with microtubule assembly or function (2, 7). Asulam also inhibits 7,8-dihydropteroate synthetase, an enzyme involved in folic acid synthesis which is needed for purine nucleotide biosynthesis (5,8). (For more details see page 14.)
Symptomology: Chlorosis in young leaves and plant stunting, followed by necrosis. Growing points usually are killed by 1-2 wk after treatment, whereas mature leaves senesce more slowly.
Absorption/translocation: Readily absorbed by foliage when POST-applied; less so by roots when soil-applied. Foliar absorption rate is increased by use of a wetting agent or oil adjuvant, but is decreased by low temperature and low humidity following treatment. Maximum foliar penetration occurs between 25 and 35 C. Asulam is both xylem and phloem mobile (6) and translocates to the growing points following uptake by roots or leaves. In certain perennial grasses, foliar-applied asulam translocates to the root system, killing dormant rhizome buds.
Metabolism in plants: Asulam apparently is metabolized in tolerant species (4).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Weakly to moderately adsorbed by soil.
K_{oc}: Average is 40 mL/g for the acid (9); ranges from 60-120 mL/g across different soils for the Na salt
Transformation:
Photodegradation: Calculated half-life with simulated sunlight was 1.5 h of natural sunlight equivalents in water at pH 9 or on soil
Other degradation: An actinomycete fungi has been found capable of growing on a nutrient medium containing asulam as the sole source of carbon.
Persistence: Typical field half-life is 7 d (9), but varies from 2.5-7 d
Lab experiments: Half-life was 8-28 d, depending on soil characteristics
Mobility: Medium to high mobility; leaching potential is very low, however, because of rapid degradation
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade asulam sodium salt unless otherwise indicated.

Acute toxicity:

Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; rat, >2000 mg/kg; 4-h inhalation LC$_{50}$ rat, >19 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, yes

Subchronic toxicity:

90-d dietary rat: NOEL >2000 mg/kg/d; no abnormal clinical symptoms

Chronic toxicity:

24-mo dietary, mouse: NOEL NA; no effects at 713 mg/kg/d (5000 mg/kg)

24-mo dietary, rat: Systemic NOEL 50 mg/kg/d (1000 mg/kg); oncogenic NOEL 50 mg/kg/d (1000 mg/kg)

6-mo dietary, dog: NOEL 60 mg/kg/d

Teratogenicity:

Rat: NOEL >2000 mg/kg/d; not teratogenic

Rabbit: NOEL maternal >750 mg/kg/d, fetal >1500 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL fetal >1250 mg/kg/d (>25,000 mg/kg), maternal >50 mg/kg/d (>1000 mg/kg); not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Dominant lethal, negative

DNA damage/repair: UDS, negative

Mammalian cell transformation: C3H/10T ½ negative

Wildlife:

Mallard duck oral LD$_{50}$, >4000 mg/kg; Partridge oral LD$_{50}$, >2600 mg/kg; Pheasant oral LD$_{50}$, >4000 mg/kg; Bluegill sunfish 96-h LC$_{50}$, >3000 mg/L; Harlequin fish 96-h LC$_{50}$, >1700 mg/L; Channel catfish 96-h LC$_{50}$, >5000 mg/L; Goldfish 96-h LC$_{50}$, >5000 mg/L; Rainbow trout 96-h LC$_{50}$, >5000 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Synthesized from sulfanylamide

Purification of technical: NA

Analytical methods: Residues can be determined using HPLC with a Spherisorb S5 ODS 1 column and pH 3 buffer/methanol (75.25 v/v) solvent. Also, see ref. 3.

Historical: Herbicidal properties were first described by May & Baker in 1965. First reported in 1965 (1).

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Cottrell and Heywood. 1965. Nature 207:655.
2. Fedtke, C. 1982. Biochemistry and Physiology of Herbicide Action. Springer-Verlag, New York.
3. GUardigli, A. et al. 1984. Pages 197-217 in G. Sweig and J. Sherma, eds., Analytical Methods for Pesticides and Plant Growth Regulators, Vol, XIII. Academic Press.
4. Harper and Appleby, 1984. Weed Res. 24:93.
5. Kidd, B. R. etal. 1982. Plant Sci. Lett. 26:211.
6. Singh and Muller. 1979. Weed Res. 19:171.
7. Sterrett and Fretz. 1975. HortScience. 10:161.
8. Veeraselaram, P. et al. 1981. Pestic. Sci. 12:325.
9. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

atrazine

CAS #: 1912-24-9 **5$^{(C_1)}$**

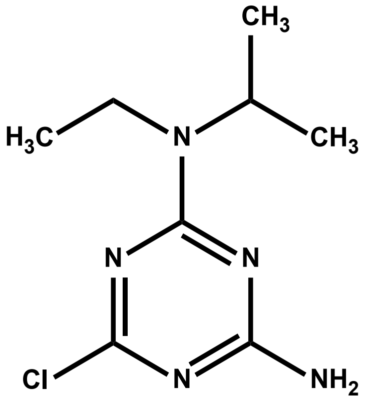
6-chloro-*N*-ethyl-*N*-(1-methylethyl)-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: atrazine (ANSI, BSI, ISO, WSSA)
Other name(s): G-30027; 2-chloro-4-ethylamino-6-isopropylamino-*s*-triazine; 2-chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine; 6-chloro-N^2-ethyl-N^4-isopropyl-1,3,5-triazine-2,4-diamine (IUPAC)
Trade name(s): A-PLUS; AMEXINE; ATRAZINE; ATRED; AATREX® NINE-O; BOXER; BULLET®; CONQUEST; GUARDSMAN®; GESAPRIM; GIFFEX; LADDOCK®; LARIAT®; LIBERTY ATZ; MALERMAIS; MARKSMAN®; PRIMOLEO; SIMAZAT; VECTAL; VEGFRU-SOLARO; VOROX GRANULAT 371; X-SIPRIM; ZEAPHOS
Chemical family: chloro-*s*-triazine; chlorotriazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
atrazine



Molecular formula: $C_8H_{14}ClN_5$
Molecular weight: 215.69 g/mole
Description: White, crystalline
Density: 0.363 g/mL (20 C)
Melting point: 175-177 C
Boiling point: NA
Vapor pressure: 3.87×10^{-5} Pa (25 C); 1.91×10^{-4} Pa (30 C); 8.0×10^{-4} Pa (40 C); 2.0×10^{-3} Pa (50 C); 5.6×10^{-2} Pa (75 C); 1.01 Pa (100 C); 12.93 Pa (125 C); 12.12 Pa (150 C); Henry's Law constant, 2.48×10^{-9} atm m^3/mole
Stability: Decomposed by UV light; hydrolytically stable at pH 5, 7, and 9 in buffered water; weak hydrolysis at 70 C in water at pH 7, but hydrolysis rates increase at lower or higher pH
Solubility:

water 33 mg/L (pH 7, 22 C)
organic solvents g/100 mL (20 C):
chloroform 5.2
diethyl ether 0.21
DMSO 18.3
ethyl acetate 2.8
methanol 1.8
n-pentane 0.023

pK_a: 1.7 (21 C) (weak base)
K_{ow}: 481 (25 C, distilled water)

HERBICIDAL USE

Atrazine can be applied as follows: early preplant, PPI, PRE, and POST at 1.1-2.2 kg ai/ha in corn and sorghum; PRE at 0.5-3.36 kg ai/ha in fallow; PRE at 1.1 kg ai/ha on roadsides; PRE or POST at 0.45-4.5 kg ai/ha in sugarcane (as single or multiple applications); PRE at 2.2-4.4 kg ai/ha on macadamia nuts, conifers, and certain established turf species; and POST-directed at 2.2-4.4 kg ai/ha on guava. Atrazine controls many broadleaf weeds including pigweed spp., morningglory spp., jimsonweed, wild buckwheat, mustard spp., ragweed spp., smartweed spp., and cocklebur, as well as certain grass weeds such as barnyardgrass and foxtail spp.

USE PRECAUTIONS

Fire hazard: All formulated products are aqueous or dry and are non-flammable with low electrical conductivity. Atrazine technical is non-combustible; flash point is >93 C.
Corrosiveness: Atrazine technical and formulated products are non-corrosive to equipment and metal surfaces.
Storage stability: Stable over several years; slight sensitivity to natural light and extreme temperatures
Cleaning glassware/spray equipment: Washing or flushing with water
Emergency exposure: May cause temporary eye or skin irritation. Repeated skin contact may cause skin sensitization. Wash skin with soap and water. Flush eyes with water. If ingested, induce vomiting or lavage stomach. No specific antidote is available, but ingestion of an aqueous slurry of activated charcoal may help inactivate the herbicide.
Incompatibilities: Compatible with most other pesticides and fertilizers; no incompatibilities known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Symptoms begin with interveinal chlorosis of the leaves and yellowing of their margins. Further chlorosis and necrosis follows in susceptible plants. Older leaves are more damaged than new growth. Browning of leaf tips can occur. Root growth is not affected.
Absorption/translocation: Absorbed through roots from soil applications and translocated to shoots predominately in the xylem; readily absorbed into leaves from POST applications with essentially no basipetal translocation out of treated leaves; surfactants or oil adjuvants increase rate and amount of absorption into foliage
Metabolism in plants: Glutathione (GSH) conjugation rapidly detoxifies atrazine in leaves of tolerant species such as corn and sorghum having high levels of GSH and active GSH transferase. GSH attacks the Cl carbon.

Benzoxazinone (DIMBOA)-catalyzed hydrolysis, producing hydroxy atrazine, occurs in roots of some species such as corn (but not sorghum) and contributes substantially to detoxification for soil-applied atrazine. *N*-dealkylation of side chains occurs at relatively low rates in most plant species, contributing significantly to detoxification only in susceptible or moderately susceptible species (such as peas and wheat) lacking appreciable rates of GSH conjugation or hydrolysis.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Over 60 species worldwide have developed triazine-resistant biotypes. Those studied at the genetic level have an altered *psbA* gene coding for a glycine in place of a serine on the D1 protein on which the atrazine binding site is located. Thus, triazines cannot bind efficiently to the D1 protein and do not block photosynthetic electron transport (2). A velvetleaf biotype from MD is tolerant to atrazine by an alternative mechanism, that of higher GSH transferase activity and faster GSH conjugation of atrazine.

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to soil; adsorption increases at lower pH

K_{oc} and K_d: Average K_{oc} is 100 mL/g (3); K_{oc} 39 mL/g and K_d 0.2 mL/g for a sand with 0.9% OM, 2.2% clay, and pH 6.5; Koc 70 mL/g and K_d 0.79 mL/g for a sandy loam with 1.9% OM, 16.8% clay, and pH 7.5; K_{oc} 155 mL/g and K_d 0.73 mL/g for a loam with 0.8% OM, 9% clay, and pH 6.7; K_{oc} 87 mL/g and K_d 2.46 mL/g for a clay with 4.8% OM and pH 5.9

Transformation:

Photodegradation: Half-life was 335 d in water at 12-45 C and pH 7 with natural light; major degradation products after 15 d were hydroxy atrazine [4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazine-2(1*H*)-one] (2.6% of applied) and *N*-deethylated atrazine (6-chloro-*N*-(1-methylethyl)-1,3,5-triazine-2,4-diamine) (2.89%). Half-life was 45 d on a sandy loam soil at 25 C and pH 7.5 under artificial light; major products after 30 d were *N*-deethylated atrazine (13.3%) and *N*-deethyl-*N*-demethylethyl atrazine (11.9%). Photodegradation moderately contributes to dissipation in the field, particularly under prolonged lack of rainfall when atrazine remains on the soil surface.

Biological degradation: Half-life was 146 d for aerobic and 159 d for anaerobic microbial metabolism in loam soil at 25 C under laboratory conditions. Metabolites were formed at low levels and were *N*-deethylated atrazine and *N*-demethylethylated atrazine (6-chloro-*N*-ethyl-1,3,5-triazine-2,4-diamine). Biological degradation moderate contributes to dissipation in the field. Recently, reports have been published regarding enhanced degradation in fields that have had continual atrazine applications (4).

Non-biological degradation: Soil hydrolysis rates are slow at high pH (pH 7.5-8), but hydrolysis becomes the major contributor to degradation at lower pH (pH 5.5-6.5), producing hydroxy atrazine.

Persistence: Average field half-life is 60 d (3). Most rotational crops can be planted 1 yr after application of atrazine at selective rates, except under an arid or semiarid climate. Persistence is increased by higher soil pH as well as by cool, drysoil conditions. Continual atrazine use may significantly reduce field persistence (4).

Mobility: In field experiments conducted in corn grown in Georgia, Minnesota, and California, no quantifiable atrazine residues (LOD = 50 μg/kg) were found below 30 cm.

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade atrazine unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 3090 mg/kg; Dermal LD_{50} rabbit, >3100 mg/kg; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, none

AATREX 4L: Oral LD_{50} male rat, 1886 mg/kg, female rat, 1075 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >2.38 mg/L; Skin irritation rabbit, mild; Eye irritation rabbit, mild

AATREX NINE-O: Oral LD_{50} rat, 1600 mg/kg; Dermal LD_{50} rabbit, >10,200 mg/kg; 4-h inhalation LC_{50} rat, >1.3 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, slight

Subchronic toxicity:

21-d dermal, rabbit: NOEL 10 mg/kg/d; body weight effects and slight decreases in mean hematology and clinical chemistry parameters at 1000 mg/kg/d

Chronic toxicity:

91-wk dietary, mouse: NOEL 1.2 mg/kg/d; increased incidence of atrial thrombi at 1500 and 3000 mg/kg; not carcinogenic

24-mo dietary, Sprague-Dawley rat: NOEL 0.7 mg/kg/d; hematopoietic effects at 1000 mg/kg; increased incidence of mammary gland tumors in females at 70, 500, and 1000 mg/kg; mode of action not considered relevant to man (EPA, IARC)

24-mo dietary, female Sprague-Dawley rat: NOEL 70 mg/kg; early onset of mammary gland tumors at 400 mg/kg; no increase in tumor incidence after 24 mo; mode of action not considered relevant to man (EPA, IARC)

24-mo dietary, Fischer-344 rats: NOEL 70 mg/kg; not carcinogenic.

12-mo dietary, dog: NOEL 3.75 mg/kg/d; slight decreases in hematology parameters and slight to moderate cardiac effects at 1000 mg/kg

Teratogenicity:

Rat: NOEL 25 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 1 mg/kg/d, developmental 5 mg/kg/d; not teratogenic

Reproduction:Rat: NOEL 50 mg/kg; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Mouse dominant lethal, negative; Chinese hamster/nucleus anomaly, negative; Mouse micronucleus, negative

DNA damage/repair: Rat hepatocytes, negative; Human fibroblasts, negative

Wildlife:

Bobwhite quail oral LD_{50}, 940 mg/kg; 8-d dietary LC_{50}, >10,000mg/kg; Mallard duck (Peking) oral LD_{50}, >10,000 mg/kg; Earthworm LC_{50} in soil, 78 mg/kg; Daphnia 24-h LC_{50}, 87 mg/L; Bluegill sunfish 96-h LC_{50}, 42 mg/L; Rainbow trout 96-h LC_{50}, 9.9 mg/L

Use classification: Restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Synthesized by successive *N*-alkylation of cyanuric chloride

Purification of technical: NA

Analytical methods: Crop samples are extracted by reflux in 80% methanol. Residues are partitioned into ethyl acetate/hexane and cleaned up on an Alumina B SepPak. Extracts are analyzed by GC with N/P detection. Soil samples are extracted with 80% acetonitrile. Samples are partitioned into dichloromethane and cleaned up on a water-deactivated alumina column. Extracts are analyzed by GC with N/P detection. Water samples are partitioned with dichloromethane, the organic layer is concentrated, and residues are determined by GC with N/P or mass selective detection. In technical samples and formulated products, GC is used for atrazine whereas HPLC is used for polar impurities and degradation products. Immunoassay procedures are available for water analysis.

Historical: Synthesis and testing of triazine compounds as herbicides began in 1952 in the Geigy laboratories in Basel, Switzerland. Atrazine was first released for experiment station evaluation in 1957 and became commercially available for use in corn in 1958. Reported in 1957 (1).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; Agriliance; Albaugh/Agri Star; BASF; Bayer CropScience; Dow AgroSciences; Drexel; DuPont Crop Protection; Helena; Micro Flo; Monsanto; Sipcom; Syngenta Crop Protection; UAP-Platte; Wilbur-Ellis

Reference(s):

1. Gysin and Knusli. 1957. Proc. 4th Intern. Congr. Crop Prot., Hamburg.
2. LeBaron and Gressel. 1982. Herbicide Resistance in Plants. John Wiley & Sons, New York.
3. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.4. Krutz, L.J. et al. 2007. Proc. South. Weed Sci. Soc., Nashville, TN.

azafenidin

CAS #: 68049-83-2

14$^{(E)}$

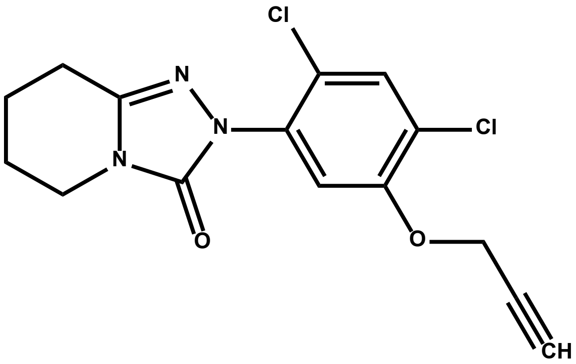
2-[2,4-dichloro-5-(2-propynyloxy)phenyl]-5,6,7,8-tetrahydro-1,2,4-triazolo[4,3-*a*]pyridin-3(*2H*)-one

NOMENCLATURE

Common name: azafenidin (ANSI, ISO, WSSA)
Other name(s): DPX-R6447; 2-(2,4-dichloro-5-prop-2ynyloxyphenly)-5,6,7,8-tetrahydro-1,2,4-triazolo[4,3-*a*] pyridin-3(2*H*)-one (IUPAC)
Trade name(s): EVOLUSO
Chemical family: triazolone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
azafenidin



Molecular formula: $C_{15}H_{13}Cl_2N_3O_2$
Molecular weight: 338.19 g/mole
Description: White powder solid
Density: 1.4 g/mL (20 C)
Melting point: 168-168.5 C
Boiling point: NA
Vapor pressure: 1.3×10^{-9} Pa
Stability: Stable to hydrolysis
Solubility: 16 mg/L (pH 7)
pK_a: None (non-ionizable)
K_{ow}: 229 (20 C)

HERBICIDAL USE

Azafenidin is currently used for weed control in vineyards, citrus, sugarcane and olive orchards, and for industrial and forest weed control (1). Azafenidin can be applied safely to the ground under citrus and olive trees at any growth stage and in vineyards from the second year after planting. Azafenidin at 240 g ai/ha can be applied either PRE alone or POST in a tank mix with a contact or POST herbicide. These applications provide excellent control of many important weeds including grasses like *Setaria*, *Digitaria*, *Poa*, and *Echinochloa* species, as well as broadleaved weeds such as *Amaranthus, Chenopodium, Malva, Brassica, Solanum* and *Portulaca* species. The recommended rate offers 60 to 180 weed free days depending on weed species. Additional testing is underway for the use of this herbicide in sugarcane, coffee, pineapple and other crops.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Technical active ingredient is not sensitive to oxidizing or reducing agents
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent.
Emergency exposure: If on skin, wash with plenty of soap and water. Get medical attention if irritation persists. If in eyes, flush with plenty of water. Call a physican if irritation persists. If inhaled, remove victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Susceptible plant species quickly exhibit necrotic symptoms and die within days of emergence.
Absorption/translocation: Absorbed through the roots and shoots of susceptible plants. Translocation in the xylem or phloem is weak explaining the limited POST activity of azafenidin on well developed weedy plants (1). However, azafenidin significantly improves the efficacy of POST herbicides such as glyphosate and increases the speed of action of contact herbicides.
Metabolism in plants: Not readily absorbed or translocated in target crops which may explain selectivity
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: No resistant weed biotypes are known to azafenidin.

BEHAVIOR IN SOIL

Sorption: Binds strongly to soil particles
K_{oc}: 298 mL/g (mean of four soils)
Transformation:
Photodegradation: Photolyzes rapidly in aquatic systems
Other degradation: Hydrolytically stable; degrades rapidly in soils via microbial degradation
Persistence: Dissipates rapidly in natural waters and is readily degraded under field conditions; half-life in four European soils ranged from 25 to 40 days
Mobility: Exhibited low mobility in four European soils. Groundwater contamination is not expected.
Volatilization: NA
Formulation effects: Environmental fate properties are unaffected by formulation.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade azafenidin.
Acute toxicity:
Oral LD_{50} rat >5000 mg/kg; Dermal LD_{50} rabbit >2000 mg/

kg; 4-h inhalation LC_{50} rat >5.3 mg/L; Primary eye irritation rabbit, non irritating; Skin irritation rabbit, negative; Skin sensitization guinea pig, negative

Subchronic toxicity:

No signs of toxicity were observed in rats exposed by dermal route to 1000 mg/kg/d technical. Slight histological changes in the liver and kidney were observed in rats treated with 6000 mg/kg or greater. NOEL (rats) 300 mg/kg/d; (dogs) 1000 mg/kg/d

Chronic toxicity: NOEL (dogs) 1000 mg/kg/d

Teratogenicity: Non-teratogenic

Reproduction: No reproductive or neonatal toxicity was observed in a two generation rat reproduction study.

Mutagenicity:

Gene mutation: Ames mutagenicity test with *Salmonella typhimurium* and *Escherichia coli* were negative.

Wildlife:

Bobwhite quail, oral LD_{50} >2500 mg/kg, 5-d dietary LC_{50} >5620 mg/kg; Mallard duck, oral LD_{50} >2500 mg/kg; 5-d dietary LC_{50} >5620 mg/kg; Daphnia, 48-h EC_{50} 38 mg/L; Bluegill sunfish, 96-h LC_{50} 48 mg/L; Rainbow Trout, 96-h LC_{50} 33 mg/L; Algal toxicity 120-h, Selenastrum c. EC_{50} 0.94 mg/L

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Discovered by DuPont de Nemours in 1992. It has been field-tested extensively in Europe. Registration is expected soon for weed control in vineyards, citrus and olive orchards as well as for industrial and forest weed control.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): DuPont Crop Protection

Reference(s):

1. Amuti, K. et al. 1997. Proc. Brighton Crop Prot. Conf. Weeds, pp. 59-66.

azimsulfuron

CAS #: 120162-55-2

$2^{(B)}$

N-[[(4,6-dimethoxy-2-pyrimdinyl)amino]carbonyl]-1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)

NOMENCLATURE

Common name: azimsulfuron (ISO)

Other name(s): IN-A8947; DPX A8947; JS-458; 1-(,6-dimethoxypyrimidin-2-yl)-3-[1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)pyrazol-5-ylsulfonyl]urea (IUPAC)

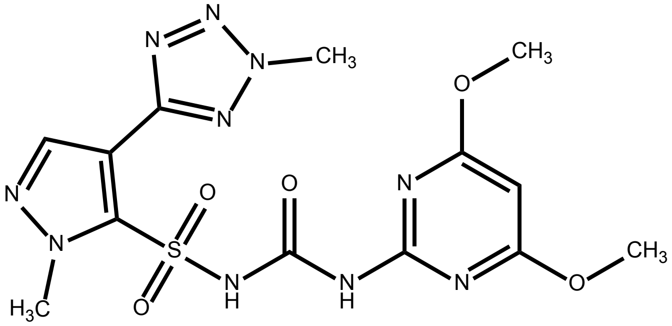
Trade name(s): GULLIUER

Chemical family: pyrazole; pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

azimsulfuron



Molecular formula: $C_{13}H_{16}N_{10}O_5S$

Molecular weight: 424.39 g/mole

Description: White solid

Density: NA

Melting point: 170 C

Boiling point: NA

Vapor pressure: 4.0×10^{-9} Pa

Stability: Hydrolysis DT_{50} (25 C); 89 d (pH 5); 124 d (pH 7); 132 d (pH 9)

Solubility:

water (20 C), 72.3 mg/L (pH 5); 1050 mg/L (pH 7); 6536 mg/L (pH 9)

Solvents in mg/L

acetone 26.4	acetonitrile 13.9
ethyl acetate 13.0	methanol 2.1
methylene chloride 65.9	toluene 1.8
hexane <0.2	

pK_a: 3.6 (weak acid)

K_{ow}: log K_{ow} = 0.646 (pH 5); -.1.37 (pH 7); -2.08 (pH 9) (25 C)

HERBICIDAL USE

Azimsulfuron is used for postemergence control of broadleaf weeds, grasses, and sedges in rice.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: NA

Storage stability: Stable when stored under normal conditions.

Emergency exposure: Skin or eye exposure, wash with water..

BEHAVIOR IN PLANT

Mechanism of action Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Chlorosis of meristem leaf tissue.

Absorption/translocation: Absorbed by roots and leaves

Metabolism in plants: *O*-demethylation of the methoxy groups on the pyrimidine ring is the primary metabolic pathway in animals and plants.

Mechanism of resistance in weeds: Resistant weeds have altered site of action

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 61-80 mL/g

Transformation:

Other degradation: Hydrolytic cleavage is faster under acidic conditions (see **Stability**)

Persistence:

Field Dissipation: Half-life 8.4 d in a rice paddy

Lab experiments: DT_{50} 11-120 d

Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade azimsulfuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; Acute dermal LC_{50} rat (4 h), 5.94 mg/L; Skin or eye irritation rabbit, no

Chronic toxicity:

24-month, rats: NOEL 1000 mg/kg diet

Mutagenicity: Non-mutagenic (Ames test)

Wildlife:

Acute 96-h LC_{50} rainbow trout, 492 mg/L; carp, >1000mg/L; Daphnia 48-h EC_{50}, >2000 mg/L; Mallard duck 8-h LD_{50}, >5620 mg/kg; Bees 48-h LD_{50}, >25 mg/bee; Earthworms LD_{50}, >1000mg/kg

Use classification: WHO Class 5

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

1. Marquez, T. Proc. Br. Crop. Prot. Conf.-Weeds, 1995, 1, 65.

beflubutamid

CAS #: 113614-08-07 $12^{(F_1)}$

2-[4-fluoro-3-(trifluoromethyl)phenoxyl]-*N*-(phenylmethyl) butanamide

NOMENCLATURE

Common name: beflubutamid

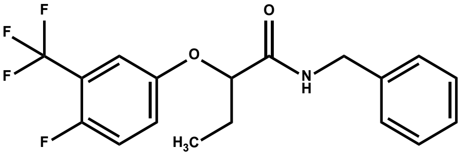
Other name(s): benfluamid; UBH-820; (*RS*)-*N*-benzyl-2-(α,α,α,4-tetrafluoro-*m*-tolyloxy)butyramide (IUPAC)

Trade name(s): NA

Chemical family: amide; phenoxybutanamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:



Molecular formula: $C_{18}H_{17}F_4NO_2$

Molecular weight: 355.33 g/mole

Description: Fluffy white powder

Density: 1.33 g/mL

Melting point: 75 C

Boiling point: NA

Vapor pressure: 1.1×10^{-5} Pa

Stability: Stable at 130 C for 5 h; stable at pH 5, 7, 9 for 5 d; relatively stable to photolysis

Solubility:

water 3.29 g/mL
acetone >60 g/L
1,2-dichloroethane >544 g/L
ethyl acetate > 571 g/L
methanol > 473 g/L
n-heptane 2.18 g/L

pK_a: None (non-ionizable)

K_{ow}: log K_{ow} = 4.28

HERBICIDAL USE

Beflubatamid is proposed for use for postemergence broadleaf weed control (*Veronica persica, Lamium amplexicaule,* and *Viola arvensis*) in rice at rates of 170-255 g ai/ha. It has potential for use in wheat, rye, barley and triticale. Is being examined as a pre-mix partner with isoproturon. Not being developed for U.S.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: NA

Storage stability: NA

Cleaning glassware/spray equipment: NA

Emergency exposure: NA

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme phytoene desaturase in carotenoid biosynthesis (more details on pages 14).

Symptomology: Foliage of sensitive plants turns white

Absorption/translocation: NA

Metabolism in plants: Same as soil

Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:

K_{oc} = 852-1793 mL/g

Transformation:

Other degradation: Degradation in soil is via biodegradation with a DT_{50} of 5.4 d. The main metabolite is 2-(4-fluoro-3-trifluormethylphenoxy) butanoic acid.

Persistence:

Field experiments: NA

Lab experiments: In water/sediment: DT_{50} = 49-64 d; in water DT_{50} = 16-20 d.

Volatilization: Minimal

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade beflubutamid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, > 5000 mg/kg; Dermal LD_{50} rat, >2000mg/kg; Acute inhalation LD_{50} rat, > 5 mg/L, Non-irritant to skin or eyes.

Subchronic toxicity:

90-d dietary, rat: NOEL 29 mg/kg/d

Teratogenicity: Rat, rabbit, Non-teratogenic

Mutagenicity: Negative in Ames test; gene mutation test, cytogenetics test, and micronucleus test

Wildlife:

Avian oral LD_{50} Bobwhite quail, >2000 mg/kg; avian dietary LC_{50} Bobwhite quail, >5200 mg/kg; earthworm LC_{50} 14d), 732 mg/kg; rainbow trout LC_{50} 96 h, 1.86 mg/L; bluegill sunfish LC_{50} 96 h, 2.69 mg/L; Daphnia acute EC_{50} 48 h, 1.64 mg/L; algae toxicity EbC_{50}, 4.45 µg/l; honeybee oral LD_{50}, > 100 µg/bee; low risk to soil microflora

SYNTHESIS AND ANALYTICAL METHODS:

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Ube Industries

Reference(s):

1. Takamura, S., T. Okada, S. Fukuda, Y. Akiyoshi, F. Hoshide, E. Funaki, and S. Sakai. 1999. UBH-820: a new selective herbicide for weed control in cereals. Proc. Brighton Conf. – Weeds. Vol. 1: 41-46.

benazolin

4-chloro-2-oxo-3(2*H*)-benzothiazoleacetic acid

CAS # Acid: 3813-05-6
Ethyl ester: 25059-80-7
Potassium salt: 67338-65-2

NC

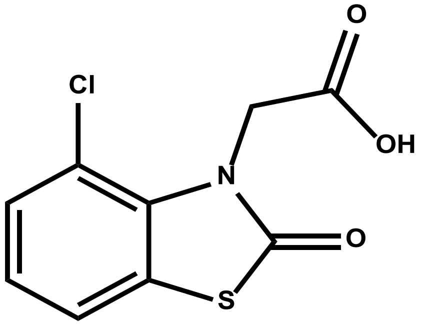
NOMENCLATURE

Common name: benazolin (ANSI, BSI, ISO, WSSA)
Other name(s): RD 7693; 4-chloro-2,3-dihydro-2-oxo-1,3-benzothiazol-3-ylacetic acid (IUPAC); 4-chloro-2,3-dihydro-2-oxobenzothiazol-3-ylacetic acid
Trade name(s): ASSET; BENASALOX; BENCORNOX; BENOPAN; BENSECAL; BENZAN; BENZAR; CATT; CHAMILOX; CORNOX CWK; CRESOPUR; GALIPAN; HERBAZOLIN; HERBITOX; LEYMIN; KEROPUR; SETTER 33; TILLOX
Chemical family: None generally accepted

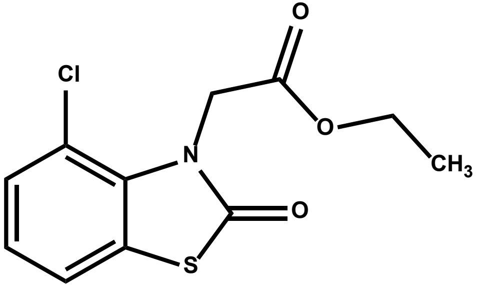
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

Benzolin acid



Benzolin ethyl ester



Molecular formula: *Acid:* $C_9H_6ClNO_3S$; *Ethyl ester:* $C_{11}H_{10}ClNO_3S$; *K salt:* $C_9H_5ClKNO_3S$
Molecular weight: *Acid:* 243.66 g/mole; *Ethyl ester:* 271.72 g/mole; *K salt:* 281.75 g/mole
Description: Colorless crystalline solid, odorless
Density: NA
Melting point: *Acid:* 189 C; *Ethyl ester:* 79.2 C
Boiling point: NA
Vapor pressure: 1.9×10^{-5} Pa (20 C)
Stability: Decomposed at 290 C
Solubility:

Acid
water 600 mg/L (20 C)
organic solvents g/100 mL (20 C):
acetone 13.2
carbon disulfide 0.05
ethanol 11.1

Ethyl ester
water 47 mg/L (20 C)
organic solvents g/100 mL (20 C):

acetone 22.9	methanol 2.9
dichloromethane 60.3	toluene 19.8
ethyl acetate 14.8	

pK_a: NA
K_{ow}: 302

HERBICIDAL USE

Benazolin can be applied at 0.28-0.42 kg ai/ha for broadleaf weed control in canola, cereals, and pastures. An oil adjuvant is needed for maximum efficacy. Benazolin is not registered in the U.S., but is used in Canada and Europe.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Concentrated solutions of the alkali metal salts at high pH are mildly corrosive to galvanized iron, tin plate, and aluminum.
Storage stability: Below pH 9-10, the Na or K salt is stable for up to 3 yr at 25 C.
Cleaning glassware/spray equipment: Clean glassware with detergent and water. Organic solvents such as acetone may be used. Equipment used for applying benazolin should not be used to apply fertilizers or other pesticides.
Incompatibilities: No known incompatibility with hard water or other pesticides. Salts are compatible with similar salt formulations of the phenoxyalkanoic acids.

BEHAVIOR IN PLANTS

Mechanism of action: NA
Symptomology: NA
Absorption/translocation: Readily absorbed through foliage and translocated primarily through the phloem.
Metabolism in plants: Rapidly metabolized in tolerant and susceptible species (2).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil
Transformation:
Photodegradation: Negligible losses
Persistence: NA
Mobility: Readily leached from soil
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade benazolin acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; mouse, >4000 mg/kg; dog, >1000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

Benazolin ethyl ester technical: Oral LD_{50} rat, >6000 mg/kg; mouse, >4000 mg/kg; dog, >5000 mg/kg; Dermal LD_{50} rabbit, >2100 mg/kg; 4-h inhalation LC_{50} rat, >5.5 mg/L; Skin irritation rabbit, none; Eye irritation rabbit, none

Subchronic toxicity:

90-d dietary, rat: NOEL ~300-1000 mg/kg/d**90-d dietary, dog:** NOEL ~300 mg/kg/d

Chronic toxicity:

24-mo dietary, rat: NOEL 300-1000 mg/kg/d

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail oral LD_{50}, >10,204 mg/kg; Japanese quail oral LD_{50}, >10,204 mg/kg; Bluegill sunfish 96-h LC_{50}, 204 mg/L

Benazolin ethyl ester technical: Bobwhite quail oral LD_{50}, >6000 mg/kg; 5-d dietary LC_{50}, >20,000 mg/kg; Japanese quail oral LD_{50}, >9709; Mallard duck, oral LD_{50}, >3000 mg/kg; 5-d dietary LC_{50}, >20,000 mg/kg; Daphnia 48-h EC_{50}, 6.1 mg/L; Bluegill sunfish 96-h LC_{50}, 2.8 mg/L; Rainbow trout 96-h LC_{50}, 5.4 mg/L

Benazolin K salt technical: Bobwhite quail oral LD_{50}, 2856 mg/kg; Japanese quail oral LD_{50}, 2856 mg/kg

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: *N*-2-chlorophenylthiourea, prepared from 2-chloroaniline, is cyclized to 2-amino-4-chlorobenzothiazole. This is converted into 4-chloro-2-oxo-benzothiazoline which is condensed with ethyl chloroacetate and the product hydrolyzed.

Purification of technical: Recrystallization from ethyl methyl ketone.

Analytical methods: GC of the methyl ester, sensitive to 10 ppb.

Historical: Properties first described in 1964 (1). Benazolin never was registered in the U.S., but has been marketed in Canada and Europe. Protected by British patent 862,226.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Leafe, E. L. 1964. Proc. 7th Brit. Weed Control Conf. p. 32.
2. Schafer and Stobbe. 1973. Weed Sci. 21:48.

benefin

CAS #: 1861-40-1

$15^{(K_3)}$

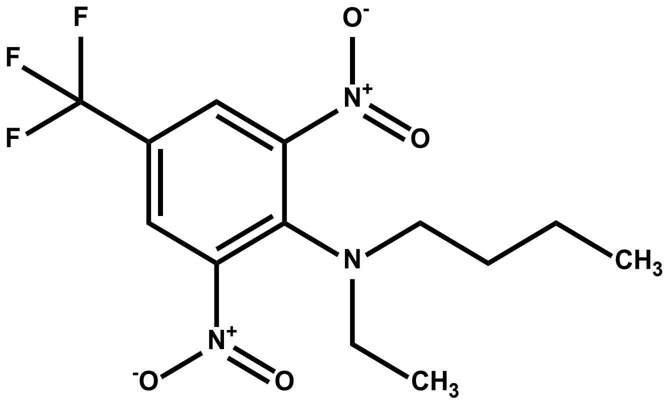
N-butyl-*N*-ethyl-2,6-dinitro-4-(trifluoromethyl)benzenamine

NOMENCLATURE

Common name: benefin (ANSI, BSI, ISO, WSSA)
Other name(s): benfluralin (BSI); EL-110; *N*-butyl-*N*-ethyl-α,α,α-trifluoro-2,6-dinitro-*p*-toluidine (IUPAC)
Trade name(s): BALAN®; BENEFEX; PRO-MATE® TURF FERTILIZER CONTAINS TEAM® PRO 0.86%; TEAM®; SPRING CRABICIDE®; XL 2G
Chemical family: dinitroaniline

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
benefin



Molecular formula: $C_{13}H_{16}F_3N_3O_4$
Molecular weight: 335.28 g/mole
Description: Yellow-orange crystalline solid, virtually odorless
Density: NA
Melting point: 65-66.5 C
Boiling point: 121-122 C (66.7 Pa); 148-149 C (933 Pa)
Vapor pressure: 1.04×10^{-2} Pa
Stability: Degraded by UV light
Solubility:
water 10.1 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C):
acetone > 50
acetonitrile >25
chloroform >50
dimethylformamide 45
dioxane 60
methanol 4
methyl ethyl ketone 58
xylene 45

pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 4.69 (8)

HERBICIDAL USE

Benefin can be applied PPI at 1.26-1.68 kg/ai/ha in alfalfa, birdsfoot trefoil, clover, lettuce, and on ornamental shrubs, ground covers, established flowers, and turf. . It primarily controls annual grasses such as barnyardgrass, broadleaf signalgrass, crabgrass spp., fall panicum, foxtail spp., and sandbur, along with certain annual broadleaf weeds including lambsquarters and pigweed spp. Benefin can be applied by conventional sprayer or impregnated on dry bulk fertilizer.

USE PRECAUTIONS

Fire hazard: Benefin technical is nonflammable
Corrosiveness: Non-corrosive
Storage stability: Shelf life is >2 yr
Cleaning glassware/spray equipment: Wash equipment with detergent and water.
Emergency exposure: Flush eyes with water for 15 min; see an ophthalmologist immediately. Call a physician or Poison Control Center.
Incompatibilities: No known incompatibilities with hard-water or other pesticides. Benefin is compatible with dry fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Mitotic disruption through inhibition of the microtubule protein tubulin (more details on page 14)
Symptomology: Most susceptible annual grasses and small-seeded broadleaf weeds fail to emerge, due to inhibition of coleoptile growth or hypocotyl unhooking. Seed germination is not inhibited. Root growth inhibition is a prominent symptom on emerged seedlings and established plants, especially in development of lateral and secondary roots. Roots appear stubby with tips becoming thickened. Grass stems such as corn may be purple near the base. The base of grass shoots swell, appearing bulbous, and the hypocotyl may swell in broadleaves. Shoots may be deformed and brittle.
Absorption/translocation: Absorbed primarily by emerging shoots (grass coleoptile, broadleaf hypocotyl or epicotyl), secondarily by seedling roots. Benefin vapor may be absorbed by foliage and cotyledons (7). Plants beyond the seedling stage readily absorb benefin into the roots, but acropetal translocation to shoots is limited. Benefin is highly lipophilic and is rapidly portioned into membranes and other lipid contents of root tissues, thereby limiting translocation.
Metabolism in plants: Benefin metabolites in plants were similar to those found in soil (1). Thus, it was suggested that the metabolites identified in plant tissue probably were absorbed from the soil following microbial degradation.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Trifluralin-resistant goosegrass from the southern U.S. also is resistant to other dinitroaniline herbicides, including benefin (2). The resistance mechanism may involve either a change in the binding site on tubulin subunits (4) or an altered microtubule-associated protein (5).

BEHAVIOR IN SOIL

Sorption: Benefin sorption to soil is significant for all soil types and greatest for soil with the highest organic matter content.
K_{oc}: Average is 10,000 mL/g

Transformation:

Photodegradation: Photolysis will contribute to the degradation of benefin in soil.

Other degradation: Laboratory degradation rates averaged 44 days.

Persistence: Field studies conducted in northern climates resulted in degradation rates comparable to the lab degradation rates..

Mobility: Negligible leaching

Volatilization: Low but significant losses if left on the soil surface

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade benefin unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >10,000 mg/kg; mouse, >5,000 mg/kg, dog >2000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50}, >2.3 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, rat: NOEL None; **90-d dietary, dog:** NOEL 5 mg/kg/d

Chronic toxicity:

24-mo dietary rat: NOEL 0.7 mg/kg/day (Males); 0.5 mg/kg/day (Females); no cumulative toxicity or serious adverse effect at ≤100 mg/kg/d

12-mo dietary, dog: NOEL 5 mg/kg/day (Females); 25 mg/kg/day (Males)

EPA classifies benfluralin in the category "suggestive evidence of carcinogenicity, but not sufficient to assess human carcinogenic potential."

Teratogenicity:

Rat: Developmental NOEL 1000 mg/kg/day,highest dose tested (HDT) no adverse effects at ≤1000 mg/kg/d

Rabbit: Developmental NOEL 225 mg/kg/day(HDT); no adverse effects at ≤225 mg/kg/d

Reproduction:

Rat:

Reproductive NOEL NA; No effects on fertility or organs of reproduction

Mutagenicity: Gene mutation: Ames, test, negative; Mouse lymphoma (L5178Y TK^+) forward mutation, negative

Structural chromosome aberration: *In vitro* ; CHO, negative;

Wildlife: Bobwhite quail oral LD_{50}, >2000 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mysid acute LC_{50}=0.043 mg a.i./L; Duckweed EC_{50} = 0.036 mg a.i/L; Rainbow trout chronic NOAEC = 0.0019 mg a.i/L; Honey bee acute contact LC50 > 101 µg/bee

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Nitration of 4-(trifluoromethyl) chlorobenzene with fuming nitric and sulfuric acid yields the 2,6-dinitro derivative. Treatment of the dinitro derivative with *N*-butyl-*N*-ethylamine produces benefin.

Purification of technical: Dissolve in hexane and pass over a Florisil chromatographic column. The first orange-colored band is benefin. Recrystallize from hexane.

Analytical methods: For benefin determination in formultated products, absorption of benefin in n-hexane can be measured at 376 nm after removal of colored impurities. Alternatively, the sample can be dissolved or extracted in chloroform, with benefin concentration determined by GC using flame ionization detection. Residue determination requires extraction of crop tissue or soil with a solvent such as methanol, removal of interfering substances on a Florisil column, and determination by GC with electron affinity detection. Test sensitivity is 5-10 µg/kg.

Historical: First described as a chemical by Q.F. Soper in U.S. patent 3,257,190 assigned to Eli Lilly and Company. First described as a herbicide in 1965 by J.F. Schwer at the Northeastern Weed Control Conference. BALAN DF registration (for agricultural uses) was transferred to Platte Chemical Company on June 17, 1993.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Dow AgroSciences; Helena; Lebanon; UAP-Platte

Reference(s):

1. Yamasue, Y. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
2. Golab, T. et al. 1970. J. Agric. Food Chem. 18:838.2.
3. Mudge, L.C. et al. 1984. Weed Sci. 32-591.
4. Vaughn, K.C. et al. 1987. Plant Physiol. 83:956.
5. Vaughn, K.C. et al. 1990. Weed Technol. 41:157.

benoxacor

CAS #: 98730-04-2 **NC**

4-(dichloroacetyl)-3,4-dihydro-3-methyl-2*H*-1,4-benzoxazine

NOMENCLATURE

Common name: benoxacor

Other name(s): CGA-154281; (*RS*)-4-dichloroacetyl-3,4-dihydro-3-methyl-2*H*-1,4-benzoxazine

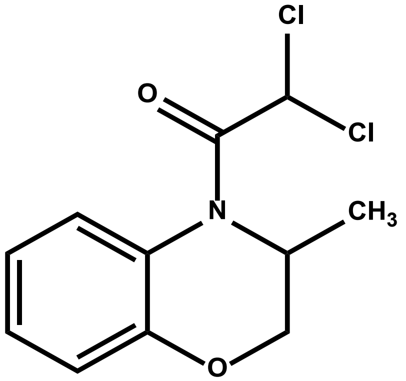
Trade name(s): TRISTAR®; DUAL II MAGNUM®; BICEP II MAGNUM® (as a safener component)

Chemical family: morpholine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

benoxacor



Molecular formula: $C_{11}H_{11}Cl_2NO_2$

Molecular weight: 260.12 g/mole

Description: Crystalline solid, colorless to pale yellow

Density: 1.47 g/mL (25 C)

Melting point: 107.6 C

Boiling point: NA

Vapor pressure: 5.9×10^{-4} Pa (20 C); 3×10^{-3} Pa (30 C)

Stability: Stable at room temperature and at (50 C)

Solubility: water 20 mg/L (20 C)

pK_a: None (non-ionizable)

K_{ow}: 392

HERBICIDAL USE

Benoxacor has no herbicidal activity but is used as a safener to protect corn from *S*-metolachlor injury that may occur during abnormally wet conditions at time of germination and emergence. It is commercially available only as a prepackage mixture and is packaged and applied in a 20:1 ratio of *S*-metolachlor to benoxacor. Thus, it can be soil-applied as an early preplant, PPI, or PRE application along with *S*-metolachlor. Benoxacor does not affect the weed control efficacy of metolachlor.

USE PRECAUTIONS

Fire hazard: Autocatalytic decomposition releases HCl at >130 C.

Corrosiveness: Technical is non-corrosive

Storage stability: Stable

Cleaning glassware/spray equipment: NA

Emergency exposure: If ingested, induce vomiting. If large amounts have been ingested and emesis is inadequate, lavage stomach. No specific antidote is available. Repeated skin contact may cause a sensitization (allergic) reaction in some individuals. Slight eye irritation may result.

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Benoxacor enhances the rate of *S*-metolachlor detoxication in corn.

Symptomology: Benoxacor does not injure plants.

Absorption/translocation: NA

Metabolism in plants: Major pathway in corn and potatoes involves reductive dechlorination with subsequent glutathione conjugation, followed by hydrolysis to yield the alcohol. The alcohol metabolite is readily conjugated to glucose. Minor pathways involve methylation of the alcohol and cyclization to the aromatic ring as well as cleavage of the amide to form the benzoxazine.

Non-antidotal biological properties: None known

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to soil

Transformation:

Photodegradation: Half-life is 6 d on soil and 1 h in water

Persistence: Typical field half-life is 2 mo

Mobility: Moderate mobility in soil

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade benoxacor unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >2 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, mouse: NOEL 500 mg/kg (NOEL male 70.7 mg/kg/d, female 99.8 mg/kg/d); decreased body weight and weight gain, hematologic effects, and liver and kidney changes at ≥2000 mg/kg

90-d dietary, rat: NOEL 100 mg/kg; decreased body weight, weight gain, and food consumption at ≥1000 mg/kg; kidney changes at ≥300 mg/kg and liver and stomach effects at 6000 mg/kg

90-d dietary, dog: NOEL 5 mg/kg/d; decreased body weight and weight gain, and liver changes at 400 mg/kg/d; decreased hematologic values in females at ≥50 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 30 mg/kg (NOEL male 3.7 mg/kg/d, female 4.7 mg/kg/d); reduced body weight gain in males at 1200 mg/kg;

increased incidence of changes in the liver and non-glandular stomach at ≥600 mg/kg

24-mo dietary, rat: NOEL 10 mg/kg (NOEL male 0.4 mg/kg/d, female 0.6 mg/kg/d); decreased body weight gain and food consumption at ≥500 mg/kg; increased incidence of changes in the liver and non-glandular stomach at ≥50 mg/kg

12-mo dietary, dog: NOEL 5 mg/kg/d; reduced body weight gain and decreased hematologic values in males, and liver and kidney changes in both sexes at ≥40 mg/kg/d

Teratogenicity:

Rat: NOEL maternal 1 mg/kg/d, developmental 100 mg/kg/d; not teratogenic; maternal toxicity, indicated by reduced body weight and weight gain at≥100 mg/kg/d; developmental toxicity at 400 mg/kg/d

Rabbit: NOEL 12.5 mg/kg/d; not teratogenic; slight maternal and developmental toxicity at 62.5 mg/kg/d

Reproduction:

Rat: NOEL 50 mg/kg in a 2-generation study; not a reproductive toxin at 1000 mg/kg (highest dose tested); reduced body weight gain in parents and pups at ≥500 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative. V79 CHO, negative

Structural chromosome aberration: Chinese hamster bone marrow/micronucleus, negative

DNA damage/repair: Rat hepatocytes/ Autoradiographic DNA repair, negative; Human fibroblasts/Autoradiographic DNA repair, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2000 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, 3600 mg/kg; Earthworm LC_{50} in soil, >1000 mg/kg; Daphnia 48-h LC_{50}, 17 mg/L; Bluegill sunfish 96-h LC_{50}, 6.5 mg/L; Carp 96-h LC_{50}, 10 mg/L; Catfish 96-h LC_{50}, 1.4 mg/L; Rainbow trout 96-h LC_{50}, 2.9 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: The multi-step synthesis begins with 2-nitrophenol and a morpholine ring closing, followed by acetylation.

Purification of technical: NA

acetonitrile/water, soil is homogenized with acetonitrile/water, and water samples are extracted with organic solvents. Extracts are cleaned-up using liquid-liquid partitioning; soil and plant extracts are further cleaned-up with a Florisil SPE column. Benoxacor residues are determined using GC with N/P detection and a capillary DB-5 column. Percentage active ingredient in benoxacor technical is determined by capillary GC on a dimethyl polysiloxane stationary phase.

Historical: Benoxacor was first synthesized in 1982 by Ciba-Geigy Ltd in Basle, Switzerland. Premix formulations with metolachlor were released for university testing in 1986. Formulations containing benoxacor were registered in 1992.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

bensulfuron-methyl

CAS #: 83055-99-6 2$^{(B)}$

methyl 2-[[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl] amino]sulfonyl]methyl]benzoate

NOMENCLATURE

Common name: bensulfuron-methyl (ANSI, BSI, ISO, WSSA)

Other name(s): DPX-F5384; methyl α-[[4,6-dimethoxypyrimidin2-yl)carbamoyl]sulfamoyl]-*o*-toluate (IUPAC)

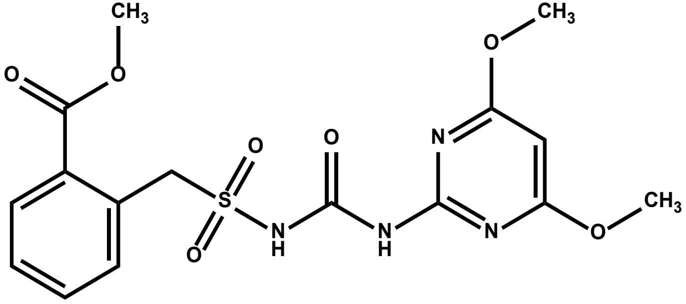
Trade name(s): LONDAX®

Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

bensulfuron-methyl



Molecular formula: $C_{16}H_{18}N_4O_7S$

Molecular weight: 410.40 g/mole

Description: White to pale yellow solid, odorless

Density: 1.41 g/mL

Melting point: 185-188 C

Boiling point: NA

Vapor pressure: 3×10^{-12} Pa (25 C)

Stability: Slowly degraded by UV light

Solubility:

water (25 C), 3 mg/L (pH 5); 120 mg/L (pH 7) (3)

Organic solvents g/100 mL (20 C):

acetone 0.138
acetonitrile 0.538
dichloromethane 1.17
ethyl acetate 0.166
n-hexane 0.000031
methanol 0.099
methylene chloride 1.17
xylene 0.028

pK_a: 5.2 (weak acid) (3)

K_{ow}: 150 (pH 5); 6.1 (pH 7); 0.1 (pH 9)

HERBICIDAL USE

Bensulfuron can be applied PRE or POST at 42-70 g ai/ha in water seeded rice, or POST at 32-42 g ai/ha 1-7 d before flooding in dry-seeded rice. It controls many emerged and submerged broadleaf weeds and sedges such as dayflower, annual arrowhead, ducksalad, eclipta, gooseweed, Mexicanweed, pickerelweed, redstem, water plantain, yellow nutsedge, rice flatsedge, and blunt spikerrush. Bensulfuron can be applied dry, in water, or mixed with dry bulk fertilizer.

USE PRECAUTIONS

Fire hazard: Technical bensulfuron and the product LONDAX are dry and non-flammable.

Corrosiveness: Technical bensulfuron and the product LONDAX are non-corrosive.

Storage stability: The product LONDAX is stable when stored free of moisture and high humidity.

Cleaning glassware/spray equipment: Wash equipment with water. Rinse with 0.5% v/v chlorine bleach or ammonia. Residues in spray equipment may redissolve in subsequent loads and injure susceptible crops, particularly when the herbicide used after bensulfuron is an emulsifiable concentrate.

Emergency exposure: Wash skin with soap and water. Flush eyes with water for at least 15 mins; consult a physician. If ingested, drink 2 glasses of water and induce vomiting; consult a physician.

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Growth of susceptible species is inhibited soon after application. Foliar chlorosis appears 3-5 d after application, followed by necrosis of the growing point. Plant death generally occurs 7-21 d after application. Certain species occasionally remain green but are stunted and not competitive with the crop. Symptom development may be delayed by > 5 d when air and water temperatures are <21 C following application.

Absorption/translocation: Rapid foliar absorption in an aqueous medium. Systemic after absorption by roots or foliage.

Metabolism in plants: The primary metabolic pathway include *O*-demethylation of the methoxypyrimidine moiety and cleavage of the sulfonylurea linkage.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Many sulfonylurea-resistant weed biotypes selected in the field by chlorsulfuron use also are resistant to other sulfonylureas including bensulfuron. The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: Moderately absorbed to OM and clay

K_{oc}: Average is 315.5 mL/g (25 C)

K_d: Ranges from 1.4 - 14 mL/g (pH 5.2 - 6.6)

1/n: 0.88-0.97 for absorption, 0.18-0.3 for desorption

Transformation:

Photodegradation: Half-life is 44 d in soil photolysis studies. Photodegradation losses likely are insignificant under field conditions.

Other degradation: Bensulfuron is metabolized by soil and aquatic microbes under aerobic and anaerobic conditions. Non-microbial hydrolysis proceeds slowly at pH 7-8, but much more rapidly at pH 5.5-6.5.

Persistence: Under field conditions, half-life in water (flooded rice field) is 5-10 d, whereas the half-life of soil-bound bensulfuron is 4-8 wk.

Mobility: Bensulfuron usually moves no deeper than the top 5-7 cm of soil.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade bensulfuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LD_{50} rat, >7.5 mg/L; Skin irritation rabbit, none; Skin sensitization Guinea pig, no; Eye irritation rabbit, none

LONDAX: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization Guinea pig, no; Eye irritation rabbit, slight-mild

Subchronic Toxicity:

90-d dietary, mouse: NOEL male 39 mg/kg/d, female 407 mg/kg/d, reduced food consumption and body weights, increased liver weights, and enlarged liver cells with changes in appearance and color at 10,000 mg/kg

90-d dietary, rat: NOEL male 475 mg/kg/d, female 407 mg/kg/d, slight reduction in red blood cell mass and increased reticulocyte counts in males at 7500 mg/kg anemia and liver weight effect at 7500 mg/kg

90-d dietary, dog: NOEL male 239 mg/kg/d, female 251 mg/kg/d; reduced body weights, increased liver weights, increased serum enzymes, and histological changes indicative of slight to minimal liver toxicity at 10,000 mg/kg

Chronic toxicity:

24-month mouse: NOEL male 455 mg/kg/d, female 460 mg/kg/d; not oncogenic; increased liver weight, enlarged liver cells, and slight histological changes indicating slight to minimal liver toxicity at 5000 mg/kg

24-month rat: NOEL 308 mg/kg/d, female 403 mg/kg/d; not oncogenic; reduced food consumption and body weights, slightly lower hemoglobin concentrations in males, increased liver weights and enlarge liver cells at 7500 mg/kg

12-month dog: NOEL male 227 mg/kg/d, female 223mg/kg/d; increased liver weights and increase serum enzymes indicated slight liver toxicity at 7500 mg/kg

Teratogenicity:

Rat: NOEL maternal 2000 mg/kg/d, fetal 500 mg/kg/d; not teratogenic; lower body weights and increased skeletal variations in fetuses at 2000 mg/kg/d

Rabbit: NOEL 300 mg/kg/d; not teratogenic; reduced maternal food consumption and body weights and other signs of material toxicity at 1500 mg/kg/d; reduced fetal weights at 1500 mg/kg/d

Reproduction:

Rat: NOEL male 20 mg/kg/d, female 22 mg/kg/d; not reproductive toxin; lower body weights for parents and offspring at 595 and 1590 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative; *E. coli* WP2 HCR, negative; CHO/HGPRT, negative

Structural chromosome aberration: Rat bone marrow/cytogenicity, negative; Human lympho-cytes/cytogenicity, negative

DNA damage/repair: SCE, weakly positive without activation; Rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LD_{50}, >5620 mg/L; Mallard duck oral LD_{50}, >2510 mg/kg; 8-d dietary LD_{50}, >5620 mg/L; Honey bee topical LD_{50}, >12.5 µg/bee; Daphnia 48-h LD_{50}, >100 mg/L; Bluegill sunfish 96-h LD_{50}, >150 mg/L; Rainbow trout 96-h LD_{50}, >150 mg/L; Channel catfish 96-h LD_{50}, >150 mg/L; Crayfish 96-h LD_{50} , >71 mg/L; Mysid shrimp 96-h LD_{50}, >130 mg/L

LONDAX: Daphnia 48-h LD_{50} , >99 mg/L; Bluegill sunfish 96-h LD_{50} , >450 mg/L; Rainbow trout 96-h LD_{50} , >450 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Product and residue analysis by HPLC

Historical: Herbicidal activity of bensulfuron was first reported by T. Yayama et al.; first marketed by Du Pont in 1989 as LONDAX

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

1. Larosa and Schloss. 1984 J. Biol. Chem. 259:8753.
2. Takeda, S. et al. 1986. Weed Res. (Japan) 31:157.
3. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
4. Schmucker, M.E. et al. 2000. Pest Managmt. Sci. 56:521-532.

bensulide

CAS #: 741-58-2 **$8^{(N)}$**

O,*O*-bis(1-methylethyl)*S*-[2-[(phenylsulfonyl)amino]ethyl] phosphorodithioate

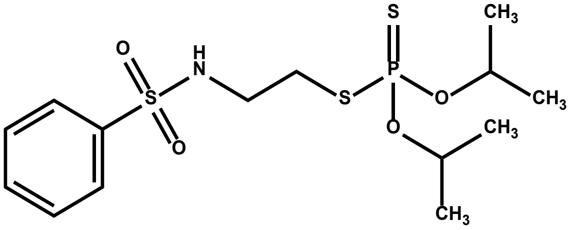
NOMENCLATURE

Common name: bensulide (BSI, ISO, WSSA)
Other names: R-4461; *O*,*O*-diiso-propyl *S*-[2-[(phenylsulfonyl)amino]ethyl]phosphorodithioate (IUPAC)
Trade names: BETASAN®; PREFAR®
Chemical family: organophosphorus; phosphorodithioates

CHEMICAL AND PHYSICAL PROPERTIES

Chemical Structure

bensulide



Molecular formula: $C_{14}H_{24}NO_4PS_3$
Molecular weight: 397.50 g/mole
Description: Colorless liquid or white crystalline solid
Density: 0.56 g/mL (@22˚C)
Melting point: 34˚C
Boiling point: NA
Vapor pressure: 1.07×10^{-4} Pa (@25˚C)
Stability: At 80˚ C degrades after induction period of 2 weeks
Solubility:

water	5.6 mg/L (25 C) (PAI)
acetone	miscible
ethanol	miscible
xylene	miscible
4-methylpentan-2-one	miscible

pK_a: None (non-ionizable)
K_{ow}: 1.65×10^4

HERBICIDAL USE

Bensulide can be applied PPI at 5.6-6.7 kg ai/ha in cucumbers, squash, pumpkins, and melons, PPI or PRE at 5.6-6.7 kg ai/ha in broccoli, Brussel sprouts, bulb onions (NM and TX), cabbage, carrots (TX only), cauliflower, lettuce, and seeded peppers, and fall PPI at 3.4 kg ai/ha in bulb onions (ID and OR). All PRE applications must be irrigated soon after application. Please read product label for detailed application information.

USE PRECAUTIONS

Fire hazard: Bensulide is non-flammable; flash point (TOC) is 157˚C, fire point is 171˚C. PREFAR 4-E is flammable. Flashpoint at 80˚C (CC method). **Corrosiveness:** Corrosive to copper, but not to mild iron, steel, tin, or brass.
Storage stability: Apparently indefinite storage life under normal ambient conditions; May be photo-degraded under certain conditions.
Emergency exposure: Follow label instructions and contact poison control center or physician as stated by the label.
Incompatibilities: Compatible with hard water and most other pesticides.

BEHAVIOR IN PLANTS

Mechanism of action: Known effects include inhibition of root elongation and cell division. (more details on page 13)
Symptomology: Root and shoot growth inhibition
Absorption/translocation: Bensulide is soil-applied and is taken up by seeds and roots with little to no translocation from roots to leaves.

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil. Inactivated in soils with high OM
K_{oc}: Average is 1433 to 4326 mL/g
Transformation:
Photodegradation: Small amounts are photo-degraded after several days
Other degradation: Slowly degraded by microbes
Photodegradation: water and soil is 200 d and 220 d, respectively.
Mobility: Not appreciably leached in soils
Volatilization: Little to no losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 360 mg/kg; Dermal LD_{50} Rat, >2000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} Rats, >1.75 mg/L; Skin irritation, mild irritant; Dermal sensitization Guinea pig, NA; Eye irritation Rabbit, Non-irritant
Wildlife:
Bobwhite quail oral LD_{50}, 1386 mg/kg; Bluegill sunfish 96-h LC_{50}, 1.4 mg/L; Rainbow trout 96-h LC_{50}, 1.1mg/L; Brown shrimp 96-h LC_{50}, 64.5 µg/L; Oyster 96-h LC_{50}, 0.24mg/L
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Manufacturer(s): Gowan Company
Source(s): Gowan Company

Reference(s):

1. Environmental Protection Agency (EPA). Reregistration Eligibility Decision (RED) for Bensulide. 2006. Interim RED document.

bentazon

CAS # Acid: 25057-89 **$6^{(C_3)}$**

3-(1-methylethyl)-1H-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide

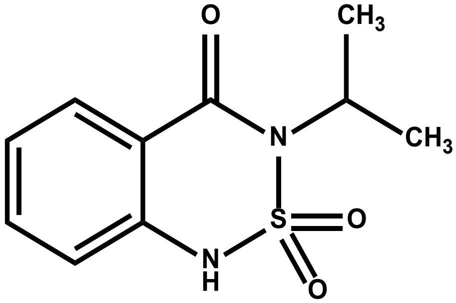
NOMENCLATURE

Common name: bentazon (ANSI, BSI, ISO, WSSA)
Other name(s): bentazone; BAS 351 07 H; BAS 3510 H; BAS 3512 H; BAS 3516 H; BAS 3517 H; BAS 3518 H; 3-isopropyl-1*H*-benzo-2,1,3-thiadiazin-4-one 2,2-dioxide; 3-isopropyl-1*H*-2,1,3-benzothiadiazin-4(3*H*)-one 2,2-dioxide (IUPAC)
Trade name(s): BASAGRAN®; BASAGRAN FORTÉ; BASAGRAN® T/O; CLEAN SWEEP®; LADDOCK®; REZULT® B; STORM®; VIPER® ADV

Chemical family: benzothiadiazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
bentazon acid



Molecular formula: $C_{10}H_{12}N_2O_3S$
Molecular weight: *Acid* 240.28 g/mole; *Na salt* 262.26 g/mole
Description: White crystalline solid, odorless
Density: 1.19 g/mL
Melting point: 137-139 C
Boiling point: 100 C (1.013×10^5 Pa)
Vapor pressure: *Acid* 9×10^{-6} Pa (20 C)
Stability: Degraded by UV light; decomposes at 200 C
Solubility:
  Acid
  water 500 mg/L (20 C)
  organic solvents g/100 mL (20 C):

acetone 120	chloroform 27
benzene 2.9	ethanol 68

  Sodium salt
  water 2,300,000 mg/L (20 C) (6)
pK_a: 3.3 (24 C) (weak acid) (7)
K_{ow}: 0.35

HERBICIDAL USE

Bentazon can be applied POST at 0.56-1.12 kg ae/ha in soybeans, beans (dry or succulent), peas, and peanuts, POST at 0.84-1.12 kg ae/ha in corn, sorghum, and rice, and POST at 1.12-2.24 kg ae/ha in established peppermint and spearmint. Bentazon is also used for established turf, ornamentals, and roadsides to control broadleaf weeds and sedges. It primarily controls annual broadleaf weeds such as velvetleaf, cocklebur, wild mustard, Venice mallow, and ragweed spp., but also controls top growth of certain perennials such as yellow nutsedge and Canada thistle.
Bentazon efficacy for certain weeds and environmental conditions is improved by adding nonionic surfactant, oil adjuvant, ammonium sulfate, or 28% urea ammonium nitrate fertilizer.

USE PRECAUTIONS

Fire hazard: BASAGRAN is non-flammable; flash point is >100 C
Corrosiveness: BASAGRAN is non-corrosive
Storage stability: Unchanged after 3 mo at 50 C. Do not allow to freeze.
Cleaning glassware/spray equipment: Wash with detergent.
Emergency exposure: Flush eyes with water for at least 15 min. Wash skin with water. If ingested, induce vomiting. Symptoms of poisoning include apathy, ataxia, prostration, tremors, anorexia, vomiting, and diarrhea.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II). (more details on page 13)
Symptomology: Chlorosis begins 3-5 d after application followed by foliar desiccation and necrosis. Foliar bronzing may occur on tolerant crops such as soybeans.
Absorption/translocation: Readily absorbed by leaves with minimal basipetal translocation following foliar application. A 4-h rain-free period after application is required for maximum bentazon efficacy (2), although this interval may be shorter with the use of certain adjuvants. Established plants grown in bentazon-treated nutrient solution culture readily absorb the herbicide into the roots and translocate it throughout the plant.
Metabolism in plants: Rapidly metabolized in tolerant species, forming glucosyl conjugates (4).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: None known.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil particles (1)
  K_{oc}: Average is 34 mL/g (6)
Transformation:
  Photodegradation: ~30% of applied bentazon degraded when exposed to light of 200-400 nm. No degradation occurred in visible light of 400-600 nm. Field half-life on soil is 4 mo. Losses due to photodegradation are negligible with field applications.
  Other degradation: Rapidly metabolized by soil bacteria and fungi and incorporated into OM by microbes. Non-microbial, non-photolytic degradation does not occur.

Persistence: Average field half-life is 20 d (6). Bentazon residues typically decline to undetectable levels within 6 wk. Bentazon has little to no soil residual activity.
Mobility: Does not leach below the plow layer
Volatilization: No losses.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade bentazon acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1100 mg/kg; mouse, 400 mg/kg; rabbit, 750 mg/kg; cat, 500 mg/kg; Dermal LD_{50} rabbit, >2500 mg/kg; 4-h inhalation LC_{50} rat, 5.1 mg/L; Skin irritation rabbit, moderate; Skin sensitization, NA; Eye irritation rabbit, moderate

BASAGRAN: Oral LD_{50} rat, 2063 mg/kg; Dermal LD_{50} rabbit, >10,000 mg/kg; 4-h inhalation LC_{50} rat, >8 mg/L; Skin irritation rabbit, mild; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL NA; LOEL 1600 mg/kg
90-d dietary, dog: NOEL NA; LOEL 3000 mg/kg

Chronic toxicity:

12-mo dietary, mouse: NOEL 10 mg/kg/d
18-mo dietary, mouse: NOEL 350 mg/kg
12-mo dietary, rat: NOEL 10 mg/kg/d
24-mo dietary, rat: NOEL 350 mg/kg
12-mo dietary, dog: NOEL 13.1 mg/kg/d

Teratogenicity:

Rat and rabbit: NOEL NA; not teratogenic

Reproduction:

Rat: NOEL NA; not a reproductive toxin

Mutagenicity: Not mutagenic

Wildlife:

Japanese quail oral LD_{50}, 720 mg/kg; Mallard duck oral LD_{50}, 2000 mg/kg; Bluegill sunfish 96-h LC_{50}, 616 mg/L; Rainbow trout 96-h LC_{50}, 190 mg/L

BASAGRAN: Bobwhite quail oral LD_{50}, 1140 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck 8-d dietary LC_{50}, >5000 mg/kg

Use classification: Restricted use for LADDOCK due to groundwater contamination concerns with atrazine; General Use for other products

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Anthranilic acid is reacted with *N*-isopropylimino sulfonyl chloride, followed by ring closure with phosgene
Purification of technical: Recrystallization
Analytical methods: Plant material is extracted with an organic solvent and bentazon residues are hydrolyzed. The extract is subjected to partition cleanup, and then methylated. Silica gel chromatography with an SPE cartridge is followed by detection of residues by capillary GC with a thermionic specific detector. Soil is extracted with an organic solvent, followed by partition cleanup, and methylation. Silica gel chromatography with an SPE cartridge is followed by detection of residues by HPLC with a fluorescence detector.
Historical: First reported in 1968 (3). Bentazon was synthesized and herbicidal activity discovered by BASF in Aktiengesellschaft, Ludwigshafen/Rhein, Germany. Bentazon was first used for control of certain 2,4-D tolerant weeds in cereal grains, and later was found to control *Cyperus* spp. in rice. The first U.S. evaluation trial occurred in 1968 at the BASF Wyandotte Agricultural Research Farm. In 1970 it was first tested for cocklebur control in soybeans. U.S. patent 3,708,277.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Arysta; BASF; United Phosphorus; Winfield

Reference(s):

1. Abernathy and Wax. 1973. Weed Sci. 21:224.
2. Doran and Andersen. 1975. Weed Sci. 23:105.
3. Fischer, A. 1968. Proc. Br. Weed Control Conf. 2:1042.
4. Otto, S. et al. 1979. Intern. IUPAC Congr. Pestic. Chem. Part 3:551.
5. Pfister, K. et al. 1974. Proc. Intern. Congr. Photosyn. 3:675.
6. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
7. Tomlin, C.L. 1994. The Pesticide Manual. Page 90. The British Crop Protection Council.

benzofenap

CAS #: 82692-44-2

$27^{(F_2)}$

2-[[4-(2,4-dichloro-3-methylbenzoyl)-1,3-dimethyl-1*H*-pyrazol-5-yl}oxy]-1-(4-methylphenyl)ethanone

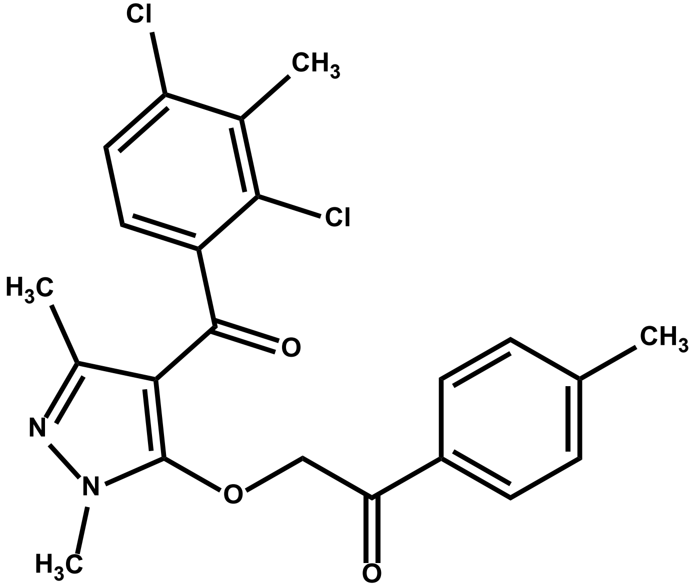
NOMENCLATURE

Common name: benzofenap (ISO)
Other name(s): MY-98; 2-[4-(2,4-dichloro-*m*-toluoyl)-1,3-dimethylpyrazol-5-yloxy]-4'-methylphenyl)ethanone (IUPAC)
Trade name(s): TAIPAH; YUKAWIDE
Chemical family: benzoylpyrazole; nicotinanalide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

benzofenap



Molecular formula: $C_{22}H_{20}Cl_2N_2O_3$
Molecular weight: 431.32 g/mole
Description: Off-white, viscuous liquid
Density: 1.09 g/mL (25 C)
Melting point: 133.1-133.5 C
Boiling point: NA
Vapor pressure: 1.3 x 10^{-6} Pa (30 C)
Stability: Stable under normal conditions
Solubility:
water, 0.13 mg/L (25 C)
xylene 69 g/L
acetone 73 g/L
n-hexane 5.6 g/L
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 4.69

HERBICIDAL USE

Benzofenap is applied to flooded rice for preemergence control of aquatic weeds such as arrowhead and seedlings of Alisma, starfruit, and water plantain at rates of 600 g ai/ha.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable under normal storage conditions.
Emergency exposure: Eye: wash with water for at least 15 min. Skin: wash affected areas with soap and water.
Incompatibilities: Strong alkalis

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme 4-hydroxyphenyl-pyruvate dioxygenase (4-HPPD) affecting carotenoid biosynthesis (more details on page 15)
Symptomology: Chlorosis and bleaching of affected foliage.
Absorption/translocation: Absorbed by roots and base of target weed species.
Metabolism in plants: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Mobility: NA
Persistence:
Field experiments: Paddy field soil DT_{50} = 38 d
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade benzofenap unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; Acute inhalation LC_{50} rats, >1.93 mg/L; mild skin sensitization.
Chronic toxicity:
24-mo dietary,rat: NOEL >5000 mg/kg
Teratogenicity: NA
Wildlife:
Dangerous to fish. Common carp LC_{50} 96 h, > 10 mg/kg; Low hazard to birds; Mallard duck LD_{50}, >2000 mg/kg; Bobwhite quail LD_{50}, >5200 mg/kg

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA**Analytical methods:** NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Mitsubishi Chemical

bifenox

CAS #: 42576-02-3 **14(E)**

methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate

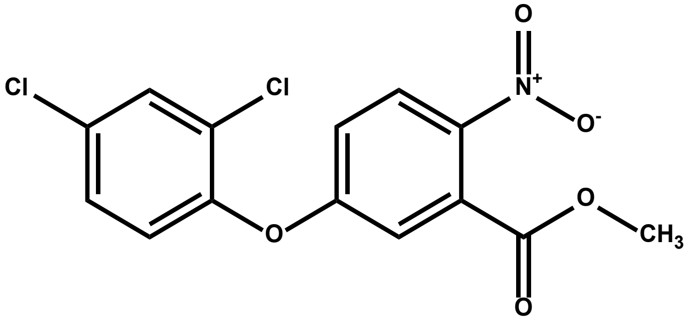
NOMENCLATURE

Common name: bifenox (ANSI, BSI, ISO, WSSA)
Other name(s): MC-4379
Trade name(s): MODOWN; FOXPRO DT; FOXTRILSUPER; LUCKY®; FIZZ®; FOX®
Chemical family: diphenylether; nitrophenylether; nitrodiphenylether

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

bifenox



Molecular formula: $C_{14}H_9Cl_2NO_5$
Molecular weight: 342.14 g/mole
Description: Crystalline solid
Density: 1.15 g/mL
Melting point: 84-86 C
Boiling point: NA
Vapor pressure: 1.3 x 10^{-9} Pa (20 C); 3.2 x 10^{-4} Pa (30 C)
Stability: Relatively stable to UV light
Solubility:
water 0.398 mg/L (25 C) (4)
organic solvents g/100 mL (25 C)

acetone 40	kerosene <1
chlorobenzene 35-40	xylene 30
ethanol <5	

pK_a: None (non-ionizable)
K_{ow}: 31,700

HERBICIDAL USE

Used on wild mustard, wild radish, and speedwell in terrestrial sites, and barnyardgrass and annual sedges in flooded paddies. It is not registered in the U.S.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: At typical dilutions in the spray tank, bifenox is virtually non-corrosive to most spray equipment materials, but is mildly corrosive to aluminum.
Storage stability: Expected shelf life is >2 yr under normal storage conditions.
Cleaning glassware/spray equipment: Clean glassware and equipment with detergent and water**Emergency exposure:** Immediately flush eyeswith water for at least 15 min. If ingested, do not induce vomiting. Poisoning symptoms in animals include hypoactivity, muscular weakness, tremors, and convulsions.

Incompatibilities: Compatible with hard water and liquid fertilizers. Incompatible with other herbicides as esters

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme proroporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Leaves of susceptible plants become chlorotic and then desiccated and necrotic within 1-2 d after a foliar application. Youngest expanded leaves of tolerant crops such as soybeans and peanuts also may show chlorosis and necrosis, especially at higher rates. Sublethal rates may produce foliar "bronzing", usually on young expanded leaves. Droplet drift may leave bleached spots or flecks on leaves. Soil applied bifenox does not affect emergence, but seedlings become necrotic and desiccated usually by 3-5 d after emergence.
Absorption/translocation: Relatively rapid absorbed by foliage. Not easily removed by rainfall. Bifenox translocates little following either foliar or soil application.
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil
K_{oc}: Average is 10,000 mL/g (estimated) (4)
Transformation:
Photodegradation: Negligible losses
Other degradation: Primarily degraded by microbes
Persistence: Typical field half-life is 7 d, although half-life can range to 14 d. Bifenox controls weeds for 6-8 wk, and residues do not injure susceptible crops planted 1 yr after application.
Mobility: Significant leaching
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade bifenox unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; mouse, >4556 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >200 mg/L; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation rabbit, none

Subchronic toxicity:

90-day dietary, rat: NOEL 300 mg/kg/d**21-d dermal, rabbit***:* NOEL NA; no adverse effects in hematologic, clinical blood chemistry, and urinalysis; no significant gross or microscopic pathology at 113 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 50 mg/kg/d

24-mo dietary, rat: NOEL 80 mg/kg/d; not carcinogenic

24-mo dietary dog: NOEL 600 mg/kg/d

Teratogenicity:

Rabbit: NOEL maternal 10-20 mg/kg/d; no major malformations at 200 mg/kg/d

Reproduction: NA

Mutagenicity: NA

Wildlife:

Mallard duck 8-d dietary $LC_{50,}$ >5000 mg/kg; Pheasant 8-d dietary LC_{50}, >5000 mg/kg; Bluegill sunfish 96-h LC_{50}, 0.64 mg/L; Rainbow trout 96-h $LC_{50,,}$0.87 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Confidential

Purification of technical: Recrystallization

Analytical methods: A gas chromatography method using a halogen-specific microcoulometric detector can be used for determination of bifenox residues in soybeans, corn, grain sorghum, rice, and small grains. The method is sensitive to 50 mg/kg.

Historical: First reported in 1973 (1). Introduced by Mobil Chemical Co. and later by Eli Lily & Co. Patents were awarded to Mobil (U.S. 3,652,645, 3,776,715 and Great Britain 1,232,368).

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience; Feinchemie

Reference(s):

1. Dest, W.M. et al. 1973. Proc. Northeast. Weed Control Conf. 27:31.
2. Duke, S.O. et al. 1991. Weed Sci. 39:465.
3. Lee and Duke. 1994. Abstr. Weed Sci. Soc. Am. 34:52.
4. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

bispyribac-sodium

CAS #: 125401-92-5 $2^{(B)}$

sodium 2,6-bis[(4,6-dimethoxy-2-pyrimidinyl)oxy]benzoate

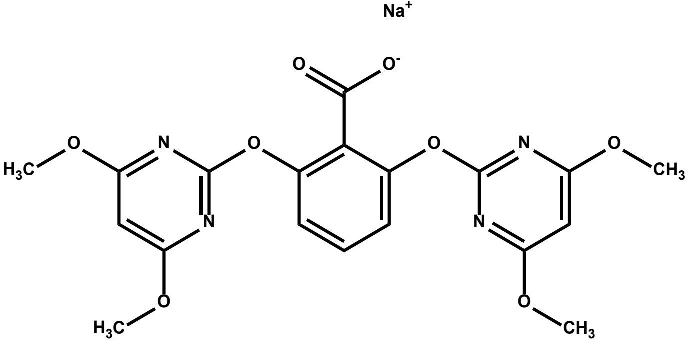
NOMENCLATURE

Common name: bispyribac-sodium (salt formulations: bispyribac-sodium)
Other name(s): KIH 2023; KUH-911; VC 1177; V-1002980S; sodium 2,6-bis(4,6-dimethoxypyrimidin-2-yloxy)benzoate (IUPAC)
Trade name(s): NOMINEE®; REGIMENT®; VELOCITY® SP
Chemical family: pyrimidinyloxybenzoic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

bispyribac



Molecular formula: $C_{19}H_{17}N_4NaO_8$
Molecular weight: 452.36 g/mole
Description: White powder
Density: 0.074 g/mL
Melting point: 223-224 C
Boiling point: NA
Vapor pressure: 5.04×10^{-9} Pa
Stability: Stable in water DT_{50} >1 yr (pH 7 and 9), 448 h (pH 4); stable in light
Solubility:

water, 73.3 g/L (20 C)
methanol 26.3 g/L
acetone 0.043 g/L (25 C)

pK_a: 3.05 (weak acid)
K_{ow}: log K_{ow} = -1.03 (23 C)

HERBICIDAL USE

Bispyribac-sodium is used for control of grasses (especially *Echinochloa spp.*) sedges, and broadleaf weeds in water seeded-rice at 15-40 g a.i./ha, wet-seeded rice at 20-40 g a.i./ha, and dry seeded rice at 20-60 g a.i./ha. It is also being examined for non-cropland weed control.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: Stable under normal storage conditions
Emergency exposure: Ingestion: give victim 1-2 glasses of water and induce vomiting.
Incompatibilities: Non-reactive with oxidizing agents.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Cessation of growth followed by chlorosis, necrosis, and plant death
Absorption/translocation: Absorbed by roots and leaves. Translocated primarily in the phloem.
Metabolism in plants: NA
Mechanism of resistance in weeds: Altered site of action

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 852-1793 mL/g
Transformation: NA
Other degradation: Very stable at pH 5-9
Persistence:
Field Experiments: DT_{50} < 10 d (flooded and upland conditions)
Lab Experiments: NA
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade bispyribac-sodium unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 4111 mg/kg, female rat, 2635 mg/kg; Dermal LD_{50} rabbit, > 2000 mg/kg; Acute inhalation rat LD_{50}, > 4.8 mg/L; Skin and eye irritation, no

Chronic toxicity:
24-mo dietary, rat: NOEL 20 mg/kg/d
12-month dog: NOEL 10 mg/kg/d

Wildlife:

Bobwhite quail and Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Pheasant 8-d dietary LC_{50}, >5000 mg/L; Bluegill sunfish and rainbow trout 96-h LC_{50}, >100 mg/L; Bees LD_{50} (oral), >200 ug/bee

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Valent
Reference(s):

1. Yokoyama M., O Watanabe, K. Kwano, and S. Shigematsu. 1993. Brighton Crop Protection Conference-Weeds-p.61-66.
2. Yokoyama M., O Watanabe, K. Yanagisawa, N. Wade, and S. Shigematsu. 1994. Weed Research, Japan 39 Supplement I, 30-33.

bromacil

5-bromo-6-methyl-3-(1-methylpropyl)-2,4(1*H*,3*H*)-pyrimidinedione

CAS # Acid: 314-40-9
Li salt: 53404-19-6

$5^{(C_1)}$

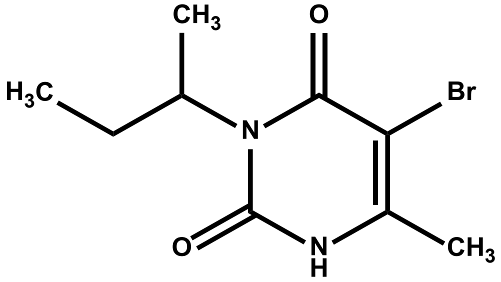
NOMENCLATURE

Common name: bromacil (ANSI, BSI, ISO, WSSA)
Other name(s): DUPONT HERBICIDE 976; (*RS*)-5-bromo-3-sec-butyl-6-methyluracil (IUPAC)
Trade name(s): BAREGROUND; BARESPOT®; BOREA; BROMAX; CYNOGAN; DIBRO; HYVAR®; KROVAR®; STAA-FREE; TOTAL™; UREABOR®; UROX "B"; UROX HX; WEED BLAST
Chemical family: uracil; substituted uracil

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

bromacil acid



Molecular formula: *Acid* $C_9H_{13}BrN_2O_2$; *Li salt* $C_9H_{12}BrLiN_2O_2$
Molecular weight: *Acid* 261.12 g/mole; *Li salt* 267.05 g/mole
Description: White, crystalline solid, odorless
Density: 1.55 g/mL (25 C)
Melting point: 158-159 C
Boiling point: NA
Vapor pressure: 4.1×10^{-5} Pa (25 C)
Stability: NA
Solubility:

Acid

water 815 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 16.7
acetonitrile 7.1
ethanol 13.4
3% sodium hydroxide 8.8
xylene 3.2

Lithium salt

water 700 mg/L (25 C) (11)
organic solvents (25 C):
acetone moderately soluble
acetonitrile moderately soluble
ethanol moderately soluble
hydrocarbons sparingly soluble

pK_a: 9.1 (weak base) (11)
K_{ow}: NA

HERBICIDAL USE

Bromacil can be applied PRE at up to 7.18 kg ae/ha per yr in citrus (multiple applications may be used), PRE at 0.9-1.8 kg ae/ha in trees, PRE at 1.8-5.4 kg ae/ha or POST at 1.8-3.6 kg ae/ha in pineapple, PRE at 1.8-5.4 kg ae/ha in non-cropland areas such as railroad rights-of-way and industrial sites, and PRE at 6.3-13.4 kg ae/ha for brush control on non-crop land.Bromacil controls many annual and perennial grasses, sedges, and broadleaf weeds including barnyardgrass, crabgrass spp., foxtail spp., bermudagrass, nutsedge spp., Florida pusley, johnsongrass, puncturevine, sandspur, and lambsquarters. Higher rates control many brush species.

USE PRECAUTIONS

Fire hazard: Technical and dry formulated products are non-flammable. The product HYVAR X-L liquid is combustible.
Corrosiveness: Alkaline liquid formulated products are corrosive to aluminum.
Storage stability: Bromacil ai is chemically stable under normal storage conditions. Exposure of HYVAR L and HYVAR X-L to air can cause some loss of water solubility.
Cleaning glassware/spray equipment: Flush equipment with water after removing nozzle tips and screens; clean tips and screens separately; clean glassware with detergent followed by acetone rinse
Incompatibilities: Bromacil formulated products are compatible with most herbicides commonly mixed with them. Certain ester formulations of phenoxy herbicides may create physical problems in the spray tank when mixed with the WP (HYVAR X). SL formulations (HYVAR L, HYVAR X-L) are incompatible with products that markedly reduce spray pH (AMS, amitrole, etc.). Precipitates form when the SL formulations are mixed with herbicides containing Ca salts.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Foliar chlorosis and necrosis.
Absorption/translocation: Readily absorbed by roots and translocated in the xylem to the leaves (6). Bromacil is less readily absorbed by leaves and stems. Surfactants enhance foliar activity. However, orange plants grown on bromacil-treated nutrient solution in sand absorbed <5% of the applied bromacil; 85% of the absorbed remained in the roots and 15% was translocated to the stem and leaves (4).
Metabolism in plants: Most of the applied bromacil was not metabolized in orange seedlings, but some 5-bromo-3-*sec*-butyl-6-hydroxy-methyluracil and an unknown minor metabolite were produced. No 5-bromouracil was detected as a metabolite of bromacil in plants.
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: Bromacil resistance has been detected in Hungary (5). A triazine-resistant Powell amaranth biotype was 16-fold more resistant to bromacil than was the susceptible biotype (1). This triazine resistance is due to an altered gene coding for the D1 protein containing the triazine binding site, which results in failure of uracil herbicides to attach to the active site. Bromacil resistance

also has been selected for in *Chlamydomonas reinhardii* (3).

BEHAVIOR IN SOIL

Sorption: Low to moderate adsorption to soil

K_{oc}: Average is 32 mL/g (11)

K_d: 0.2-1.8 mL/g

Transformation:

Photodegradation: Negligible losses

Other degradation: Microbial degradation apparently contributes to bromacil degradation (10). Bromacil is not metabolized to 5-bromouracil in soil.

Persistence: Average field half-life is 60 d (11). When used at higher rates, phytotoxic residues persist for more than 1 yr.

Field experiments: Half-life was 5-6 mo when 4.5 kg/ha were applied to a Butlertown silt loam

Mobility: Moderately mobile (9)

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade bromacil acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 5175 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >4.8 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, none; Eye irritation rabbit, mild

Subchronic toxicity: NA

Chronic toxicity:

18-mo dietary, mouse: NOEL NA; liver adenomas/carcinomas in male at 5000 mg/kg

24-mo dietary, rat: NOEL 50 mg/kg; not oncogenic; body weight effects at ≥250 mg/kg

12-mo dietary, dog: NOEL 625 mg/kg (highest level tested)

Teratogenicity:

Rat: NOEL maternal 20 mg/kg/d, fetal 75 mg/kg/d

Rabbit: NOEL maternal 100 mg/kg/d, fetal 100 mg/kg/d; not teratogenic; weight loss and resorption at 300 and 500 mg/kg

Reproduction:

Rat: NOEL 250 mg/kg in a 3-generation study; body weight effects

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: Mouse micronucleus, negative; *In vitro* cytogenetics, clastogenic

DNA damage/repair: UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck 8-d dietary LC_{50}, >10,000 mg/kg; Bluegill sunfish 48-h LC_{50}, 71 mg/L; Carp 48-h LC_{50}, 164 mg/L; Rainbow trout 48-h LC_{50}, 75 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Three recrystallizations from 95% ethanol or two from absolute ethanol.

Analytical methods: Microcoulometric GC methods of bromacil detection are sensitive to about 40 ppb (7, 8).

Historical: Substituted uracils were first described as herbicides in 1962 (2). U.S. patents 3,325,357 and 3,352,862 were awarded to Du Pont.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

1. Boydston and Al-Khatib. 1992. Weed Sci. 40:513.
2. Bucha, H. C. et al. 1962. Science 137:537.
3. Galloway and Mets. 1984. Plant Physiol. 74:469.
4. Gardiner, J. A. et al. 1969. J. Agric. Food Chem. 17:980.
5. LeBaron, H. M. 1991. Pages 27-66 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Ltd., Oxford.
6. McFarlane, J. C. et al. 1987. J. Environ. Qual. 16:372.
7. Pease, H. L. 1966. J. Agric. Food Chem. 14:94.
8. Pease, H. L. 1968. J. Agric. Food Chem. 16:54.
9. Rhodes, R. C. et al. 1970. J. Agric. Food Chem. 18:524.
10. Torgeson and Mee. 1967. Proc. Northeast. Weed Control Conf. 21:584.
11. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

bromoxynil

3,5-dibromo-4-hydroxybenzonitrile

CAS # 1689-84-5 $5^{(C_1)}$

NOMENCLATURE

Common name: bromoxynil (ANSI, BSI, ISO, WSSA)

Other name(s): M&B 10064; TORCH; 2,6-dibromo-4-cyanophenyl octanoate for the octanoate ester; 3,5-dibromo-4-hydroxybenzonitrile (IUPAC); 4-cyano-2,6-dibromophenol

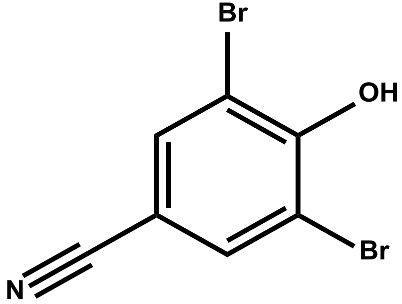
Trade name(s): BISON®; BROCLEAN®; BROMAC®; BROMINAL; BROMINEX; BROMOTRIL; BROMOX; BRONATE®; BRONATE® ADVANCED; BROZINE®; BUCTRIL®; BUCTRIL® 4 CEREALS; BUCTRIL® 4 EC; BUCTRIL® + ATRAZINE; CONNECT® 20 WSP; DOUBLE UP B+D; ECLAT; LITAROL M; MOXY®; OXYTRIL; OXYTRIL M; PARDNER®; SPRINGCLENE; STARANE* NXT; WILDCARD EXTRA

Chemical family: benzonitrile; hydroxybenzonitrile; nitrile

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

bromoxynil acid



Molecular formula: *Acid* $C_7H_3Br_2NO$; *Octanoate ester* $C_{15}H_{17}Br_2NO_2$

Molecular weight: *Acid* 276.91 g/mole; *Octanoate ester* 403.11 g/mole

Description: *Acid* Light buff to creamy powder, odorless (pure); *Octanoate ester* Cream-colored solid, characteristic odor

Density: NA

Melting point: *Acid* 190 C (technical), 194-195 C (pure); *Octanoate ester* 45-46 C

Boiling point: NA

Vapor pressure: 6.2×10^{-6} Pa (25 C)

Stability: NA

Solubility:

Acid

water 130 mg/L (20-25 C)

organic solvents g/100 mL (25 C):

acetone 17
benzene 1
cyclohexanone 17
dimethylformamide 61
ethanol 7
methanol 9
tetrahydrofuran 41

Octanoate ester

water 0.08 mg/L (20-25 C) (7)

organic solvents g/100 mL (25 C):

acetone 10
benzene 70
chloroform 80
cyclohexanone 55
dichloromethane 80
ethanol 10
xylene 70

pK_a: 4.06 (weak acid)

K_{ow}: <100

HERBICIDAL USE

Bromoxynil can be applied as follows: POST at 0.21-0.56 kg ae/ha in wheat, barley, oats, rye, and triticale; POST at 0.28-0.56 kg ae/ha in seedling alfalfa and grasses used on Conservation Reserve land; POST at 0.28-0.42 kg ae/ha in field corn, popcorn, grain sorghum, annual canarygrass, peppermint, spearmint, and onions; POST at 0.28 kg ae/ha in flax; and POST at 0.42 kg ae/ha in garlic and in turfgrasses for sod or seed. It controls many annual broadleaf weeds such as lambsquarters, nightshade spp., Pennsylvania smartweed, shepherd's-purse, wild buckwheat, kochia, cocklebur, and velvetleaf.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: Non-corrosive

Storage stability: Stable for >2 yr of storage

Cleaning glassware/spray equipment: Flush with water.

Emergency exposure: If bromoxynil technical is ingested, induce vomiting, but do not if BUCTRIL or other EC formulations are ingested.

Incompatibilities: Salt formulations can be applied in hard water at ≤600 mg/kg hardness. Ester formulations (BUCTRIL, etc.) are not affected by hard water; may be incompatible with other pesticides.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)

Symptomology: Chlorosis usually begins within 1-2 d and complete foliar necrosis develops 3-6 d after application under favorable weather conditions.

Absorption/translocation: Readily absorbed into leaves after POST application with little to no basipetal movement to other plant parts.

Metabolism in plants: Hydrolysis of the nitrile group occurred in wheat followed by production, via the corresponding amide, of a carboxyl group which may subsequently be decarboxylated (2).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Bromoxynil-resistant common lambsquarters has been detected in Germany (4). Bromoxynil-resistant transgenic plants have been developed with a bacterial gene (*bxn*) coding for a nitrilase that degrades bromoxynil (5).

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 10,000 mL/g (estimated) for the octanoate ester

Transformation: NA

Persistence: Average field half-life is 7 d

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade bromoxynil acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} weanling rat, 260 mg/kg; adult rat, 440 mg/kg; mouse, 160 mg/kg; rabbit, 335 mg/kg; Dermal LD_{50} rabbit, >3660 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, mild; Skin sensitization, NA; Eye irritation rabbit, mild

BUCTRIL: Oral LD_{50} rat, 779 mg/kg

BRONATE: Oral LD_{50} rat, 691 mg/kg

Subchronic toxicity: NA

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail oral LD_{50}, 170 mg/kg; 8-d dietary LC_{50}, 1315 mg/kg; Mallard duck oral LD_{50}, 200 mg/kg; 8-d dietary LC_{50}, 2150 mg/kg; Pheasant chick; 8-d dietary LC_{50}, 4400 mg/kg; Honey bee, non-toxic; Daphnia 48-h LC_{50}, 0.11 mg/L; Catfish LC_{50}, 0.023 mg/L; Goldfish LC_{50}, 0.17 mg/L; Rainbow trout 96-h LC_{50}, 0.1 mg/L

Use classification: All products containing atrazine are Restricted use due to groundwater contamination concerns.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Auwers and Reis (1) reported in 1896 the synthesis of halo hydroxybenzonitriles. Their procedure is outlined here, specifically for bromoxynil. *p*-hydroxybenzaldehyde is treated with bromine to obtain the 3,5-dibromo derivative, which is converted to the oxime with hydroxylamine. The oxime is treated with acetic anhydride to form 3,5-dibromo-4-acetoxybenzonitrile, which is then refluxed in 4% alcoholic NaOH to form bromoxynil.

Purification of technical: Recrystallize several times from distilled water

Analytical methods: Product analysis by GLC or by determination of bromine; residues determined by GLC of a derivative or by IR spectrometry

Historical: First synthesized in Germany in 1896 (1). U.S. patent 3,397,054 describes bromoxynil and ioxynil as herbicides. Wain et al. (6) reported the herbicidal activity of the ioxynils independently of Amchem's work. Bromoxynil development was reviewed by Heywood (3) in 1966.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; Agriliance; Bayer CropScience; Dow AgroSciences; Helena; Kwizda; Micro Flo; Syngenta Crop Protection; UAP-Platte

Reference(s):

1. Auwers and Reis. 1896. Ber. Deut. Chem. Ges. 29:2355.
2. Buckland, J. L. et al. 1973. Pestic. Sci. 4:149.
3. Heywood, B. J. 1966. Chem. In. (London). p. 1946.
4. LeBaron, H. M. 1991. Pages 27-66 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Ltd., Oxford.
5. Stalker, D. M. et al. 1988. Science 242:419.
6. Wain, R. L. et al. 1963. Nature 200:28.
7. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

butachlor

CAS #: 23184-66-9 **$15^{(K_3)}$**

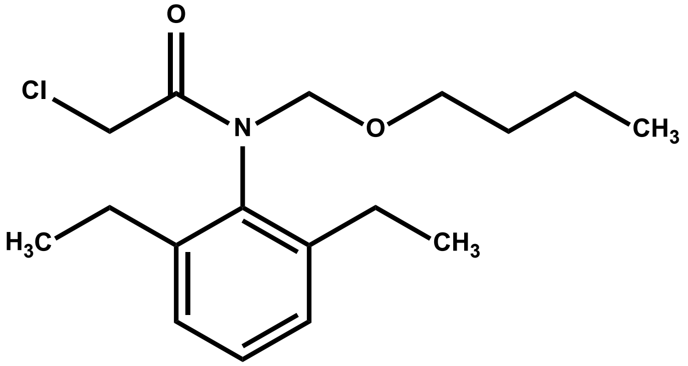
N-(butoxymethyl)-2-chloro-*N*-(2,6-diethylphenyl)acetamide

NOMENCLATURE

Common name: butachlor (ANSI, BSI, ISO, WSSA)
Other name(s): CP-53619; *N*-butoxymethyl-⟨-chloro-2',6'-diethylacetanilide; *N*-butoxymethyl-2-chloro-2',6'-diethylacetanilide (IUPAC); *N*-(butoxymethyl)-2-chloro-2',6'-diethylacetanilide; 2-chloro-2',6'-diethyl-*N*-(butoxymethyl) acetanilide
Trade name(s): AIMCHLOR; LAMBAST; MACH-MACH; WIDKIL; MACHETE
Chemical family: acetamide; acetanilide; chloroacetamide; chloroacetanilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *Butachlor*



Molecular formula: $C_{17}H_{26}ClNO_2$
Molecular weight: 311.85 g/mole
Description: Amber liquid, aromatic and slightly sweet
Density: 1.07 g/mL (25 C)
Melting point: <10 C
Boiling point: 156 C (966.65 Pa)
Vapor pressure: 6×10^{-4} Pa
Stability: Stable to UV light; decomposes at 165 C
Solubility:
water 23 mg/L (24 C)
pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

Butachlor can be soil-applied in rice for control of annual grasses and certain broadleaf weeds. It is not currently marketed in the U.S., but is used in Asia, Africa, South America, and Europe.

USE PRECAUTIONS

Fire hazard: Formulated butachlor is combustible; flash point is 114 C by open cup and 93 C by closed cup.
Corrosiveness: Butachlor is non-corrosive to no. 316 and no. 304 stainless steel, aluminum, and heresite, but corrodes steel and black iron.
Storage stability: Stable. Not sensitive to light or heat.
Cleaning glassware/spray equipment: Clean glassware with detergent; flush equipment with water
Emergency exposure: Flush skin with water; flush eyes with water; get medical attention
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Thought to be inhibition of very long chain fatty acid synthesis (VLCFA) (more details on page 14)
Symptomology: Susceptible grass and broadleaf weeds usually fail to emerge. Injury on grasses that do emerge appears as malformed and twisted seedlings. Leaves are tightly rolled in the whorl and may not unroll normally. Injured dicot crops may have cupped or crinkled leaves with a thick, leathery texture. New leaves can show a shortened midrib producing a "drawstring" or heart-shaped appearance.
Absorption/translocation: Absorbed primarily by emerging shoots (grass coleoptile, broadleaf hypocotyl or epicotyl). Some root absorption occurs. Plants beyond the seedling stage readily absor butachlor into the roots and translocate it acropetally throughout the shoots, with primary accumulation in vegetative and less in reproductive parts. Translocation in established plants is irrelevant to mechanism of action because butachlor is phytotoxic only to emerging seedlings. Translocation can occur in both xylem and phloem in established plants but primarily xylem.
Metabolism in plants: Metabolized rapidly, primarily to polar, water-soluble metabolities (3).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Adsorbed by soil colloids
K_{oc}: Average is 700 mL/g (1)
Transformation:
Photodegradation: Not appreciably photo-degraded
Other degradation: Primarily degraded by microbes
Persistence: Average field half-life is 12 d (1). Weed control efficacy persists 6-10 wk depending on soil characteristics, temperature, and moisture.
Mobility: NA
Volatilization: Minimal losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade butachlor unless otherwise indicated
Acute toxicity:
Oral LD_{50} rat, 2000 mg/kg; Dermal LD_{50} rabbit, 13,100 mg/kg; 4-h inhalation LC_{50} rat, >4.7 mg/kg; Skin irritation rabbit, moderate; Skin sensitization, guinea pig; yes; Eye irritation rabbit, slight
Subchronic toxicity: NA
Chronic toxicity:
18-mo dietary, mouse: NOEL NA; not oncogenic**24-mo**

dietary, rat: NOEL ≤100 mg/kg/d; oncogenic
12-mo dietary, dog: NOEL 5 mg/kg/d
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife:
Bobwhite quail oral LD_{50}, 10,000 mg/kg; 8-d dietary LC_{50}, 6597 mg/kg; Mallard duck oral LD_{50}, 4640 mg/kg; 8-d dietary LC_{50}, 10,000 mg/kg; Daphnia 48-h LC_{50}, 2.4 mg/L; Bluegill sunfish 96-h LC_{50}, 0.44 mg/L; Carp 96-h LC_{50}, 0.32 mg/L; Rainbow trout 96-h LC_{50}, 0.52 mg/L; Crayfish 96-h LC_{50}, 26 mg/L
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Butoxymethylation of the appropriate acetanilide
Purification of technical: Fractional distillation
Analytical methods: Macroanalysis can be done using total chlorine and infrared methods. Microanalysis can be done with GC. Residues determined by GC.
Historical: First reported in 1970 (2). Butachlor was commercialized in 1971 as MACHETE for international rice and barley markets. U.S. patents 3,442,945, 3,547,620, and others were awarded to Monsanto Company.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Monsanto
Reference(s):

1. Augustijn-Beckers, P.W.M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Baird and Upchurch, 1970. Proc. South. Weed Control Conf. 23:101.
3. Böger, P., B. Matthes, and J. Schmalfuss. 2000. Pest. Manag. Sci. 56:497-508.

butafenacil

CAS #: 134605-64-4 **$14^{(E)}$**

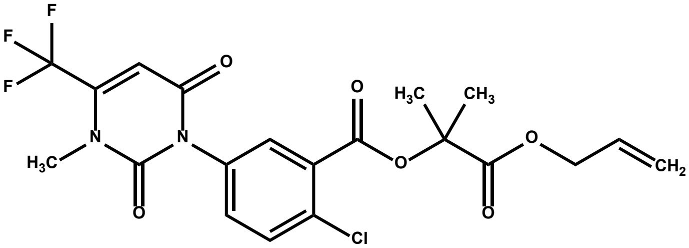
1,1-dimethyl-2-oxo-2-(2-propenyloxy)ethyl 2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-trifluoromethyl)-1(2*H*)-pyrimidinyl]benzoate

NOMENCLATURE

Common name: butafenacil (ISO 1750 accepted)
Other name(s): CGA-276854; 1-(allyloxycarbonyl)-1-methylethyl 2-chloro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoate (IUPAC)
Trade name(s): INSPIRE™; REBIN™; LOGRAN B-POWER
Chemical family: pyrimidindiones; uracil

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
butafenacil



Molecular formula: $C_{20}H_{18}ClF_3N_2O_6$
Molecular weight: 474.82 g/mole
Description: White fine powder, slight odor, colorless
Density: 1.37 g/mole
Melting point: ~113 C
Boiling point: 270-300 C
Vapor pressure: 7.4×10^{-9} Pa (25 C)
Stability: Hydrolytically stable in an acidic medium; very labile in alkaline medium (pH 9)
Solubility: 10 mg/L (25 C)
pK_a: None (Non-ionizable)
K_{ow}: 1540 ±(64) (25 C)

HERBICIDAL USE

Under development as a cotton defoliant with contact herbicidal activity. Other crops and uses are under consideration.

USE PRECAUTIONS

Fire hazard: Combustible
Corrosiveness: Avoid contact with skin, eyes, and clothing.
Storage stability: No stability problems; stable up to 250 C
Cleaning glassware/spray equipment: Use carbonated or soapy water
Emergency exposure: In case of indisposition, place patient in a well ventilated area and protect from hypothermia. In case of suspected poisoning: immediately call a physician.
Incompatibilities: Protect from light and humidity; store separately from feed, food and stimulants

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Post-emergence applications of butafenacil lead to rapid chlorosis followed by necrosis in leaves and stems of susceptible weed species, which then die within a few days. Initial herbicidal symptoms, however, are already observed within a few hours after treatment. After a preemergence application of butafenacil, cotyledons and the first leaves of emerging susceptible plants become chlorotic immediately and then die.
Absorption/translocation: Butafenacil applied post-emergence is taken up mainly by the leaves and stems. Butafenacil applied pre-emergence is absorbed mainly by the shoots of emerging seedlings, but some uptake can also occur through the roots. The uptake of the compound under preemergence conditions is dependent on the availability of butafenacil in the soil solution. The addition of the appropriate surfactant significantly increases uptake, but translocation remains limited.
Metabolism in plants: NA
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: Soil adsorption coefficient K_d = 2.1 mL/g, moderate to strong adsorption to Collombey soil.
Transformation:
Photodegradation: Direct photolysis has no practical relevance for the degradation of butafenacil.
Other degradation: Butafenacil is mainly degraded by microbial activity.
Persistence: Butafenacil is rapidly degraded in soil (half-life less than 2 d) and in water-sediment systems (half-life less than 4 d).
Mobility: Butafenacil adsorbs strongly to moderately to soil. Butafenacil will not accumulate in soil or surface waters and will not leach to groundwater. Some of the soil metabolites of butafenacil are mobile and have the potential to leach to shallow groundwater, however, these metabolites are of no environmental or toxicological concern.
Volatilization: Low vapor pressure, butafenacil can be classified as non-volatile.

TOXICOLOGICAL PROPERTIES

Butafenacil and its formulations are unlikely to present any acute risk to humans when used under normal precautionary measures for crop protection agents.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA**Purification of technical:** NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

butroxydim

CAS #: 138164-12-2 **1**$^{(A)}$

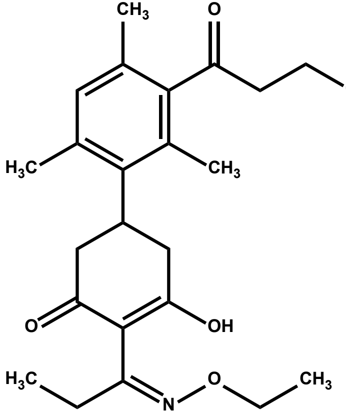
2-[1-(ethoxyimino)propyl]-3-hydroxy-5-[2,4,6-trimethyl-3(1-oxobutyl)phenyl]-2cyclohexen-1-one

NOMENCLATURE

Common name: butroxydim (BSI, ISO 1750)
Other name(s): fenoxydim; butralkoxydim; butryloxydim; ICI-A0500; (5RS)-5-(3-butyryl-2,4,6-trimethylphenyl)-2-[(EZ)-1-(ethoxyimino)propyl]-3-hydroxycyclohex-2-en-1-one (IUPAC)
Trade name(s): FALCON®; FUSION®; FACTOR
Chemical family: cyclohexanedione; cyclohexane-dione oxime; cyclohexenone; cyclohexene oxime.

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
butroxydim



Molecular formula: $C_{24}H_{33}NO_4$
Molecular weight: 399.5 g/mole
Description: Off-white powdery solid
Density: 1.2 g/mL (25 C)
Melting point: 80.8 C
Boiling point: NA
Vapor pressure: 1 x 10^{-6} Pa (20 C)
Stability: Hydrolysis DT_{50} 10.5 d (pH 5, 25 C); > 240 d (pH 7, 25 C); stable (pH 9, 25 C)
Solubility:

water 6.9 mg/L (20 C)
organic solvents (20 C)

dichloromethane > 500 g/L	acetone 450 g/L
toluene 480 g/L	acetonitrile 380 g/L
methanol 90 g/L	hexane 30 g/L

pK_a: 4.36 (weak acid)
K_{ow}: log K_{ow} = 1.9 (pH 7, 25 C)

HERBICIDAL USE

Post-emergence herbicide for the control of annual grasses in many broadleaf crops; Rate(s): 25-75 g/ha

USE PRECAUTIONS

Fire hazard: Combustible; burns with flames. Keep away from sources of ignition.
Corrosiveness: Non-oxidizing
Storage stability: Keep container tightly closed in a cool, well-ventilated place. Keep away from sources of ignition.
Emergency exposure: On ingestion, do not induce vomiting. Wash mouth out with water seek medical advice immediately. On eye contact, wash eyes with water for 15 min.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)
Symptomology: Growth ceases within a few days of application with young and actively growing tissues affect first. Leaf chlorosis and eventually necrosis develop within 1 to 3 wks of application.
Absorption/translocation: Readily absorbed into roots and leaves
Metabolism in plants: Rapidly metabolized in plants
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Due to insensitive form of ACCase or enhanced metabolism by the plant.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 6 to 1270 mL/g; stronger adsorption in low pH soils
Transformation:
Photodegradation: Photodegradation in water
Other degradation: Aerobic soil degradation
Persistence: DT_{50} is 9 d
Mobility: At low pH, substance has moderate mobility; at high pH it is highly mobile
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade butroxydim material unless otherwise indicated.
Acute toxicity:
Oral LD_{50} female rat, 1635 mg/kg, male rat, 3476 mg/kg; Dermal LD_{50} rat, > 2000 mg/kg; LC_{50} (4-h) inhalation rat, > 2.99 mg/L; Skin irritant rabbit, moderate; Eye irritant rabbit, mild; Skin sensitization guinea pigs, no
Chronic toxicity:
24-month dietary to rat: no carcinogenic effects.
Teratogenicity:
Rat: NOEL 45 mg/kg/day
Wildlife:
Mallard ducks oral LD_{50}, > 2000 mg/kg; 5-d dietary LC_{50}, > 5200 mg/kg; Bobwhite quail, 1221 mg/kg; bobwhite quail, 5200 mg/kg; honey bee LD_{50} (contact), > 200 µg/bee; LC_{50} for rainbow trout, > 6.9 mg/L; bluegill sunfish, 8.8 mg/L, EC_{50} daphnia magna, > 3.7 mg/L
Use classification: Toxic, dangerous to the environment

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: First sold in 1995.

MANUFACTURER(S) AND INFORMATION SOURCES

Industry source(s): Syngenta Crop Protection

butylate

CAS #: 2008-41-5 **$8^{(N)}$**

S-ethyl bis(2-methylpropyl)carbamothioate

NOMENCLATURE

Common name: butylate (BSI, ISO, WSSA)

Other name(s): R-1910; *S*-ethyl diisobutylthiocarbamate (IUPAC)

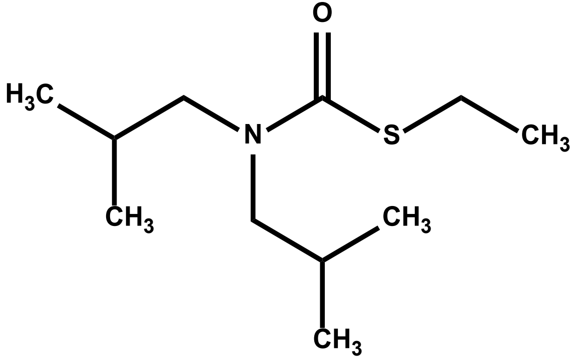
Trade name(s): SUTAN® 6.7-E; SUTAN®+; SUTAZINE

Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

butylate



Molecular formula: $C_{11}H_{23}NOS$

Molecular weight: 217.37 g/mole

Description: Clear colorless liquid, aromatic odor

Density: 0.94 g/mL (25 C)

Melting point: NA

Boiling point: 108 C (6.66×10^2 Pa)

Vapor pressure: 1.73 Pa (25 C)

Stability: Stable at 53 C for 2 wk; stable to moisture; stable in water at pH 5, 7, and 9 (25 C); stable in the presence of steel, aluminum, and zinc; photode-graded in aqueous solution exposed to sunlight (94% loss in 48 h)

Solubility:

water 44 mg/L (20 C); 45 mg/L (22 C)

organic solvents (20 C):

miscible in acetone, acetonitrile, ethanol, ethyl acetate, *n*-hexane, kerosene, methylisobutyl ketone, toluene, 4-methylpentan-2-one, xylene

pK_a: None (non-ionizable)

K_{ow}: 14,000 (25 C)

HERBICIDAL USE

Butylate can be applied PPI at 3.5-6.9 kg ai/ha in corn (field, sweet, silage, and popcorn) for control of many annual grasses such as foxtail spp., barnyardgrass, fall panicum, seedling johnsongrass, and shattercane as well as purple and yellow nutsedge and a few broadleaf weeds. Butylate must be incorporated soon after application to prevent volatilization losses. Liquid formulations can be mixed with certain liquid fertilizers, impregnated on dry bulk fertilizers, or applied through irrigation water.

USE PRECAUTIONS

Fire hazard: SUTAN+ 6.7-E is non-flammable, but has moderate fire hazard; flash point is 110 C (TOC) and fire point is 132 C.

Corrosiveness: Technical is non-corrosive to stainless and carbon steel, and to aluminum.

Storage stability: Apparently indefinite storage life under normal ambient conditions. Photosensitivity is indeterminate.

Cleaning glassware/spray equipment: Clean glassware with solvent followed by water; flush equipment with water.

Emergency exposure: Flush skin with water for at least 15 min; get medical attention if irritation occurs. Flush eyes with water for at least 15 min; get medical attention. If ingested, drink several glasses of water but do not induce vomiting.

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)

Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Injury on corn (when applied without safener) appears as malformed and twisted seedlings. Leaves are tightly rolled in the whorl and may not unroll normally. Injured dicot crops may have cupped or crinkled leaves with a thick, leathery texture. New leaves are puckered with a “drawstring effect”.

Absorption/translocation: Absorbed by roots and coleoptiles of emerging grass seedlings, although absorption by the coleoptile, especially near the coleoptilar node, is probably most important. Primary absorption in emerging susceptible broadleafs appears to occur in the hypocotyl hook. Butylate and other thiocarbamates appear to translocate basipetally and acropetally in emerged plants and probably basipetally in emerging seedlings. Translocation likely is unimportant in herbicidal action because butylate is absorbed very near its site of inhibition.

Metabolism in plants: Based on its structural similarity with other thiocarbamate herbicides, butylate in tolerant crops probably is first oxidized to the butylate sulfoxide and then detoxified by conjugation with glutathione (homo-glutathione in legumes). Subsequent cleavage of amino acids from the glutathione tripeptide and conjugation with malonate yields the malonyl-3-thiolactic acid conjugate of butylate. Butylate half-life in tolerant plants appears to be a few h or less. Butylate residues disappear from stems and leaves of corn 7-14 d after treatment.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: None known.

BEHAVIOR IN SOIL

Sorption: Weakly to moderately adsorbed to soil**K_{oc}:** Average is 400 mL/g (5)

Transformation:

Photodegradation: Half-life is 280 d on soil

Other degradation: Metabolized rapidly by microbes

Persistence: Average field half-life is 13 d (5). Buty-late generally provides ~4-7 wk of weed control and does not injure crops the following yr.

Field experiments: Half-life in several soils was 1.5-3 wk

Lab experiments: Half-life was 3 wk in a loam soil at 21-27 C

Mobility: In leaching columns with loamy sand (≤5% clay, <5% OM), butylate moved to ≤38 cm with 20 cm of applied water, while the water moved to 86 cm. In columns filled with clay loam (20-33% clay, <12% OM), butylate moved to ≤15 cm with 20 cm of applied water, while the water moved to 61 cm.

Volatilization: Substantial losses when applied to wet soils without incorporation, but little loss occurs after application to dry soil.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade butylate unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 4659 mg/kg; female rat, 5431 mg/kg; male guinea pig, 1659 mg/kg; Dermal LD_{50} rabbit, 1659 mg/kg; 4-h inhalation LC_{50} rat, 4.64 mg/L; Skin irritation rabbit, mild edema and mild-moderate erythema; Skin sensitization guinea pig, none-moderate; Eye irritation rabbit, none

SUTAN 6E: Oral LD_{50} male rat, 5366 mg/kg; female rat, 3878 mg/kg; Dermal LD_{50} rabbit, >4640 mg/kg

Subchronic toxicity:

90-d dietary, rat: NOEL 32 mg/kg/d

90-d dietary, dog: NOEL 40 mg/kg/d

Chronic toxicity:

24-mo dietary, rat: NOEL 50 mg/kg/d; not oncogenic at up to 320 mg/kg/d

Teratogenicity: NA

Reproduction: NA

Mutagenicity:

Gene mutation: Ames test, negative

Wildlife:

Bobwhite quail 7-d dietary LC_{50}, 40,000 mg/kg; Honey bee, nontoxic; Bluegill sunfish 96-h LC_{50}, 6.9 mg/L; Rainbow trout 96-h LC_{50}, 4.2 mg/L

SUTAN 6E: Bobwhite quail 7-d dietary LC_{50}, 27,000 mg/kg; Bluegill sunfish 96-h LC_{50}, 7.2 mg/L; Mosquito fish 96-h LC_{50}, 8.5 mg/L; Rainbow trout 96-h LC_{50}, 5.2 mg/L.

Use classification: General Use for SUTAN+, but Restricted use for SUTAZINE+ and SUTAZINE+ 18-6G due to groundwater contamination concerns with atrazine.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Ethyl chlorothiolformate is reacted with diisobutyl amine and base

Purification of technical: NA

Analytical methods: Extracts are cleaned-up on several types of columns and detected by GC, thermal conductivity, flame ionization, or mass spectrometry.

Historical: First reported in 1962 (3). Introduced by Stauffer Chemical Company. U.S. patent 2,913,327.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Helm Agro US; Syngenta Crop Protection

Reference(s):

1. Casida, J. E. et al. 1974. Science 184:573.
2. Fuerst, E. P. 1987. Weed Technol. 1:270.
3. Gray, R. A. et al. 1962. Proc. North Cent. Weed Control Conf. 19:19.
4. Gronwald, J. W. 1991. Weed Sci. 39:435.
5. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

cacodylic acid

dimethylarsinic acid

CAS # Acid: 75-60-5
Sodium salt: 124-65-2

NC

NOMENCLATURE

Common name: cacodylic acid (WSSA)

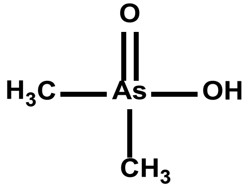
Other name(s): **Note: Cacodylic acid concentrations are expressed in cacodylic acid equivalents, but all formulated products listed here actually contain Na cacodylate + cacodylic acid in a ratio of ~5.8:1. Dimethylarsenic acid (IUPAC); hydroxydimethylarsine oxide

Trade name(s): ACME®; BROADSIDE; CACODYLATE; COTTON-AIDE HC; DILIC; DMAA; LEAF ALL; HERB-ALL; MONCIDE; LIQUID EDGER; QUICK PICK™; RAD-E-CATE 25; SIVISAR 510; WEED-ENDER

Chemical family: arsenical; organic arsenical

CHEMICAL AND PHYSICAL PROPERTIES

Cacodylic acid



Molecular formula: *Acid:* $C_2H_7AsO_2$;
Na salt: $C_2H_6AsNaO_2$

Molecular weight: *Acid:* 138.00 g/mole;
Na salt: 159.98 g/mole

Description: White crystalline powder; a common form of cacodylic acid technical, however, is a 390 g ae/L aqueous solution containing Na cacodylate + cacodylic acid in a 5.8:1 ratio, referred to below as the 390 g/L aqueous technical.

Density: *Acid:* 1.1 g/mL; *Na salt:* 0.8 g/mL; *390 g/L aqueous technical:* 1.32 g/mL

Melting point: 196-198 C

Boiling point: >200 C

Vapor pressure: NA

Stability: Stable at high and low temperatures; Stable under simulated sunlight.

Solubility:

water 102,000 mg/L (20 C)

organic solvents g/100 mL (25 C):

ethanol 20.6	*n*-hexane 0.102
ethyl ether insoluble	methanol 3.63

pK_a: *Acid:* 6.17 (25 C); *Na salt:* 6.21 (25 C)

K_{ow}: <0.028 (25 C)

HERBICIDAL USE

Cacodylic acid can be foliar-applied at 8.33-9.1 kg ae/ha in industrial sites and other noncrop areas, and at 0.91-1.14 kg ae/ha as a preharvest desiccant in cotton. It also can be applied at 8.33 kg ae/ha to destroy weeds and existing turf before lawn renovation. Cacodylic acid is non-selective and controls top growth on numerous annual and perennial weed species.

USE PRECAUTIONS

Fire hazard: All formulated products are aqueous and non-flammable.

Corrosiveness: All formulated products are mildly corrosive.

Storage stability: All formulated products are completely stable in storage.

Cleaning glassware/spray equipment: Flush with water.

Emergency exposure: Wash eyes and skin with water for 15 min. If ingested, induce vomiting. Call a physician if exposed. Symptoms include burning of throat, colicky stomach pains, and garlicky odor of breath or skin. Treat as for general arsenic poisoning.

Incompatibilities: Compatible with hard water

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Photosynthesis and dry matter production in rice was reduced when treated with cacodylic acid (3).

Symptomology: NA

Absorption/translocation: Translocated in both apoplast (including xylem) and symplast (including phloem), although symplastic transport following a foliar application is weak, perhaps due to rapid phytotoxic action in the leaves (2).

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil

K_{oc}: Average is 1000 mL/g (estimated) (1)

Transformation:

Photodegradation: No losses

Persistence: Average field half-life is estimated at 50 d (1). However, residues are strongly adsorbed to soil and do not injure subsequently planted crops.

Mobility: Low mobility in soil. Cacodylic acid does not leach appreciably.

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with dry technical grade cacodylic acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 2756 mg/kg; Dermal LD_{50} rabbit, 2000 mg/kg; 4-h inhalation LC_{50} rat, 4.9 mg/L; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation rabbit, yes.

Subchronic toxicity: NA

Chronic toxicity:

24-mo dietary, mouse: NOEL male, <200 mg/kg; female, <40 mg/kg; slightly decreased body weight and food intake, and increased water intake at 500 mg/kg

12-mo dietary, dog: NOEL 16 mg/kg/d; diarrhea, vomiting, and slightly reduced body weight gain at 40 mg/kg/.

Teratogenicity:

Rat: NOEL 12 mg/kg/d; decreased food intake, decreased body weight gain, and smaller fetus size at 36 mg/kg/d

Rabbit: NOAEL fetal 3-12 mg/kg/d; decreased food intake and body weights at 48 mg/kg/d

Reproduction:

Rat: NOEL NA; no impairment of reproduction and no adverse effects on growth and development of offspring at 3, 21, and 147 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative with or without microsomal enzymes; Mouse lymphoma, negative with and without metabolic activation

Structural chromosome aberration: Mouse micronucleus, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, >61.6 mg/L; Rainbow trout 96-h LC_{50}, >152 mg/L

CACODYLATE 3.25: Bobwhite quail oral LD_{50}, >2250 mg/kg; Honey bee oral LD_{50}, 100 µg/bee; Bluegill sunfish 96-h LC_{50}, >133 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Sodium cacodylate [$(CH_3)_2As(ONa)_2$] is synthesized in a 5-step reaction as follows:

$As_2O_3 + 6NaOH \rightarrow 2Na_3AsO_3 + 3H_2O$

$Na_3AsO_3 + CH_3Cl \rightarrow CH_3AsO(ONa)_2 + NaCl$

$CH_3AsO(ONa)_2 + SO_2 \rightarrow CH_3AsO + Na_2SO_4$

$CH_3AsO + 2NaOH \rightarrow CH_3As(ONa)_2 + H_2O$

$CH_3As(ONa)_2 + CH_3Cl \rightarrow (CH_3)2As(ONa)_2 + H_2O$

Cacodylic acid $(CH_3)_2AsO(OH)$ is then made by acidification of sodium cacodylate:

$(CH_3)_2As(ONa)_2 + HCl \rightarrow (CH_3)_2AsO(OH) + NaCl$

Also, see Initial Scientific Review of Cacodylic Acid, December 1975, U.S. Environmental Protection Agency.

Purification of technical: NA

Analytical methods: Titration with HCl, using an auto-end point titrometer.

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Luxembourg; Monterey; PBI Gordon; UAP-Platte

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Bromilow and Chamberlain. 1991. Pages 245-284 *in* R. C. Kirkwood, ed., Target Sites for Herbicide Action. Plenum Press, New York.
3. Marin, A. R. et al. 1993. J. Plant Nutr. 16:865.

carbetamide

CAS #: 16118-49-3

$23^{(K_2)}$

(2*R*)-*N*-ethyl-2-[[(phenylamino)carbonyl]oxyl]propanamide

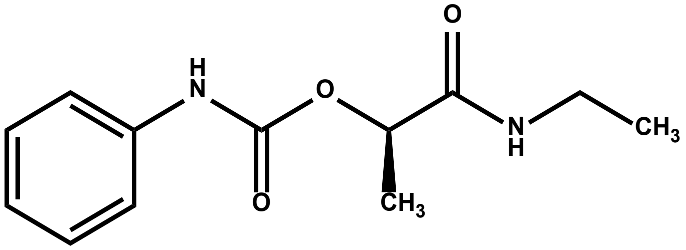
NOMENCLATURE

Common name: carbetamide (ISO approved)
Other name(s): RP-11561; (*R*)-1-(ethylcarbamoyl)ethyl carbanilate (IUPAC)
Trade name(s): CARBETAMEX®; PRADONE®; KOMBI; LEGURAME®
Chemical family: carbanilate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

carbetamide



Molecular formula: $C_{12}H_{16}N_2O_3$
Molecular weight: 236.27 g/mole
Description: Colorless crystals
Density: NA
Melting point: 119 C
Boiling point: NA
Vapor pressure: 3×10^{-7} Pa (20 C)
Stability: Stable under normal storage conditions
Solubility:
- water, 3.5 g/L (20 C)
- acetone 900 g/L
- dimethylformamide 1500 g/L
- ethanol 850 g/L
- methanol 1400 g/L
- cyclohexane 0.3 (g/L)

pK_a: None (non-ionizable)
K_{ow}: log $K_{ow} \sim 1.7$

HERBICIDAL USE

Carbetamide is a POST herbicide for the control of annual grasses including volunteers, blackgrass, meadow grasses, and wild oat and selected broadleaf weeds in winter oil-seed rape, kale seed, cabbage, swede, sugar beet, winter field beans, Lucene, sainfoin, spring greens and red and white clovers at 2 kg ai/ha.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: Non-corrosive
Storage stability: Stable under normal storage conditions.
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits cell division and microtubule polymerization (more details on page 15)
Symptomology: Growth of susceptible plants is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by slow, general foliar chlorosis and necrosis.
Absorption/translocation: Absorbed principally by roots, but can be absorbed by leaves.
Metabolism in plants: Rapidly metabolized in plants
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No specific resistant known

BEHAVIOR IN SOIL

Sorption:

K_d ranges from 0.10 mL/g (0.01 % OM, pH 6.6) to 7.93 mL/g (16.9% OM, pH 6.8)

Transformation: NA
Persistence: DT_{50} of approximately 1 mo
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade carbetamide unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >2000 mg/kg; Dermal rabbit LD_{50}, >500 mg/kg; 4-h inhalation LC_{50} rat, >0.13 mg/L; Skin irritation rabbit, none; Eye irritation rabbit, none

Chronic toxicity:

90-d dietary, dog: NOEL 3200 mg/kg/d (5000 mg/kg); not oncogenic

Wildlife:

Bobwhite quail oral LD_{50}, >2000 mg/kg; Honey bee topical, non-hazardous; Daphnia 48-h LC_{50}, 36.5 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L

Use classification: General use; WHO Class III, EPA Class IV

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience; Feinchemie

carfentrazone-ethyl

CAS #: 122836-35-5

$14^{(E)}$

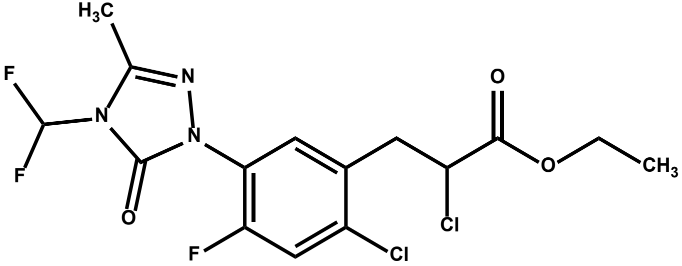
ethylα2-dichloro-5-[4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl]-4-fluorobenzenepropanoate

NOMENCLATURE

Common name: carfentrazone-ethyl (ANSI, ISO, WSSA)
Other name(s): F-8426; ethyl (*RS*)-2-chloro-3-[2-chloro-5-(4-difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl)-4-fluorophenyl]propionate (IUPAC)
Trade name(s): ADDIT™; AIM™; AURORA™; ORATIO®, PLATFORM™; QUICKSILVER™; SHARK™; SPOTLIGHT™; TEAMWORK®
Chemical family: aryl triazinone; triazolone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
carfentrazone-ethyl



Molecular formula: $C_{15}H_{14}Cl_2F_3N_3O_3$
Molecular weight: 412.20 g/mole
Description: Various yellow liquid
Density: 1.46 g/mL (20 C)
Melting point: -22.1 C
Boiling point: 350-355 C (1.013 x 10^5 Pa)
Vapor pressure: 1.6 x 10^{-5} Pa (25 C); 7.2 x 10^{-6} Pa (20 C)
Stability: Stable at room temperature
Solubility:
water 12,000 mg/L (20 C); 22,000 mg/L (25 C); 23,000 mg/L (30 C)
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 3.36

HERBICIDAL USE

AIM™ 40 WG and SHARK™ 40 WG are POST applied contact, non-residual herbicides used at 4-36 g ai/ha for control and suppression of a wide spectrum of broadleaved weeds in fallow/preplant burndown systems, field corn, seed corn, popcorn, corn silage, sweet corn, grain sorghum, rice, soybean, wheat, barley, and oats. Carfentrazone-ethyl is highly effective against a number of weed species resistant to herbicides such as imidazolinones and the sulfonylurea acetolactate synthase (ALS) inhibitors. POST-directed and layby applications of AIM 40 WG at 13.5-54 g ai/ha and defoliation applications at 18-27 g ai/ha in cotton are pending registrations. POST broadcast applications of AIM 40 WG at 28-56 g ai/ha for vine and leaf desiccation is pending registration as a harvest aid in potato.

USE PRECAUTIONS

Fire hazard: Technical and formulated carfentrazone-ethyl are non-flammable. the technical, 40 WG and 2 EC formulations, respectively. The 2 EC formulation is moderately combustible. When heated above the flash point, the 2 EC releases vapors which, when mixed with air, can burn or be explosive.
Corrosiveness: All formulated carfentrazone-ethyl products are non-corrosive.
Storage stability: Good stability. Store in cool, dry place and avoid excess heat. Store in original containers only. Keep out of reach of children and animals. Do not contaminate water, food or feed by storage or disposal.
Cleaning glassware/spray equipment: Clean glassware and equipment with a solution of soap and water. Avoid contamination of water by cleaning of equipment or disposal of wastes.
Emergency exposure: If ingested, drink 1-2 glasses of water. Do not induce vomiting or give anything by mouth to an unconscious individual. Contact a medical doctor. If inhaled, remove to fresh air. If breathing discomfort occurs, contact a medical doctor. For skin and eye exposure, wash with plenty of soap and water or flush with water for at least 15 min., respectively. If irritation occurs or persists get medical attention.
Incompatibilities: Carfentrazone-ethyl has been found to be physically compatible with most commercially available herbicides.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme proroporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Plants treated with the herbicide carfentrazone-ethyl become necrotic and die shortly after treatment. Initial symptoms are observed within hours and death within a few days.
Absorption/translocation: Carfentrazone-ethyl is absorbed rapidly by foliage of treated plants, with rainfastness achieved within 15 min. of application. Symplastic phloem movement is assumed to be limited, based on rapid foliar desiccation, although some species are well-controlled even without total spray coverage.
Metabolism in plants: Carfentrazone-ethyl is rapidly metabolized in plants (wheat, corn, soybean, potatoes). Carfentrazone-ethyl undergoes a series of reactions including hydrolysis, oxidative decarboxyl-ation, dechlorination, hydrogenolysis and conjugation. Principal metabolites include: carfentrazone-ethyl-chloropropionic acid, 3-desmethyl-carfentrazone-ethyl - chloropropionic acid, -hydroxymethyl-carfentrazone-ethyl-chloropropionic acid, and carfentrazone-ethyl-propionic acid. Crop residue studies (wheat, barley, corn, rice, sorghum, and soybean) showed that the rapid degradation of carfentrazone-ethyl

and its metabolites. No residues were found in any grain or soybean seed.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Development of weed resistance to this herbicide has not been observed.

BEHAVIOR IN SOIL

Sorption: Not strongly adsorbed to sterile soils. In non-sterile soils, carfentrazone-methyl is rapidly converted to carfentrazone-ethyl propionic acid. The free acid has low soil adsorption characteristics.

K_{oc}: 750 mL/g (25 C) for carfentrazone-ethyl

K_{oc}: 15-25 mL/g (25 C, pH 5.5) for carfentrazone acid

Transformation:

Photodegradation: Carfentrazone-ethyl is not susceptible to photodecomposition or volatility following application to soil.

Other degradation: Based on laboratory tests, loss of carfentrazone-ethyl in soil appears to be primarily by microbial degradation.

Persistence: Carfentrazone-ethyl is non-persistent in the soil. Carfentrazone-ethyl rapidly degrades by microbial degradation and hydrolysis to carfentrazone-ethyl-propionic acid which is low to moderately adsorbed to soil. The DT_{50} carfentrazone-ethyl-propionic acid is less than 0.1 d.

Mobility: Neither carfentrazone-ethyl, the short-lived free acid nor any of the other metabolites of carfentrazone-ethyl leach in the soil or contaminate ground water.

Volatilization: Carfentrazone-ethyl is non-volatile.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade carfentrazone-ethyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat (both sexes), >5000 mg/kg; Dermal LD_{50} rat (both sexes), >4000 mg/kg; Primary eye irritation rabbit, minimal; Skin irritation rabbit; non-irritating; Skin sensitization guinea pig, non-sensitizing

Carfentrazone-ethyl 40 WG: Oral LD_{50} rat (both sexes), >5000 mg/kg; Dermal LD_{50} rat (both sexes), >4000 mg/kg; Inhalation toxicity (4h) rat (both sexes), LC_{50} >5.72 mg/L; Primary eye irritation rabbit, minimal; Skin irritation rabbit, non-irritating; Skin sensitization guinea pig, non-sensitizing

Carfentrazone 2 EC: Oral LD_{50} rat, 4077 mg/kg; Dermal LD_{50} rat, >4000 mg/kg; Inhalation toxicity (4h) rat (both sexes), LC_{50} >6.31 mg/L; Primary eye irritation rabbit, minimal; Skin irritation rabbit, non-irritating

Subchronic toxicity:

90-d dietary, mouse: NOEL male and female 4000 mg/kg (571 mg/kg/d)

90-d dietary rat: NOEL male 4000 mg/kg female 4000 mg/kg (284 mg/kg/d)

90-d dietary, dog; NOEL male and female 1500 mg/kg/d.

Oncogenicity:

Mouse: NOEL male >7000 mg/kg (1091 mg/kg/d) (highest dose tested), female >7000 mg/kg (1302 mg/kg/d) (highest dose tested)

Reproduction:

Rabbit: NOEL > 150 mg/kg/d; developmental > 300 mg/kg/d (highest dose tested)

Rat: NOEL 100 mg/kg/d; developmental, >300 mg/kg/d (highest dose tested)

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HORT, negative

Structural chromosome aberration: Mouse micronucleus, negative; in vitro cytogenetics (human lymphocytes), negative; in vitro cytogenetics (Chinese hamster lung cells), increases in chromosome aberrations were only observed in the absence of S9 mix at dose levels exceeding solubility (>2000 mg/mL) with precipitating test material present.

Wildlife:

Non-hazardous to birds, no effects were observed in bobwhite quail (>2250 mg/kg) or mallard duck (>5620 mg/kg). Carfentrazone-ethyl and its formulations do not present a hazard to mammals mg/kg/body weight. Carfentrazone-ethyl and its formulations are of low acute (35 μg/bee) and topical (>200 μg/bee) toxicity to honeybees. Carfentrazone-ethyl is low to moderately toxic to fish and Daphnia. Under field conditions, however, carfentrazone-ethyl does not present a hazard to aquatic organisms because of low use rates and its rapid hydrolysis to less toxic metabolites.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Carfentrazone-ethyl was introduced in 1992 by the FMC Corporation. It was first field tested in 1993 through 1997. It is covered by U.S. Patent 5,125,958.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Agriliance; FMC

Reference(s):

1. Van Saum, W.A. et al. 1993. Proc. Brighton Crop Prot. Conf. – Weeds, pp. 19-22.
2. Martringe, M. et al. 1989. Biochem. J. 260:231.
3. Wilkowki, D.A. and Halling, B.P. 1989. Plant Physiol. 90:1239.

chlorimuron-ethyl

CAS #: 90982-32-4 $2^{(B)}$

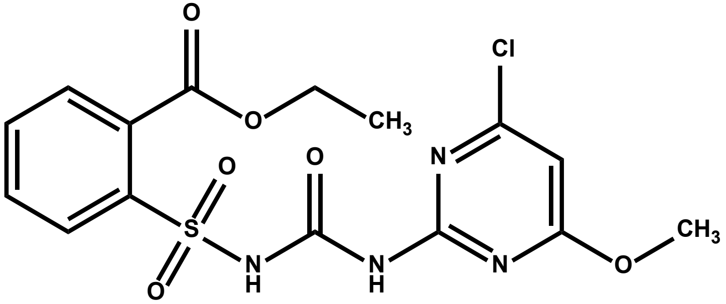
ethyl 2-[[[[(4-chloro-6-methoxy-2-pyrimidinyl)amino)]
carbonyl]amino]sulfonyl]benzoate

NOMENCLATURE

Common name: chlorimuron-ethyl (ANSI, BSI, ISO, WSSA)
Other name(s): DPX-F6025; ethyl 2-(4-chloro-6-methoxypyrimidin-2-ylcarbamoylsulfamoyl)benzoate (IUPAC)
Trade name(s): CANOPY®; CANOPY® EX; CANOPY® XL; CLASSIC®; MATADOR®; SYNCHRONY®; SYNCHRONY® XP; VALOR® XLT
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
chlorimuron-ethyl



Molecular formula: $C_{15}H_{15}ClN_4O_6S$
Molecular weight: 414.82 g/mole
Description: White solid
Density: NA
Melting point: 185-187 C
Boiling point: NA
Vapor pressure: 5×10^{-10} Pa (25 C)
Stability: NA
Solubility:
water (25 C), 11 mg/L (pH 5); 450 mg/L (pH 6.5); 1200 mg/L (pH 7)
organic solvents g/100 mL (25 C):
acetone 0.705
acetonitrile 0.31
benzene 0.08
ethanol 0.039
n-hexane 0.0006
methanol 0.074
methylene chloride 1.53
xylene 0.028
pK_a: 4.2 (weak acid)
K_{ow}: 320 (pH 5); 2.3 (pH 7)

HERBICIDAL USE

Chlorimuron-ethyl can be applied POST at 8.8-13.1 g ai/ha or preplant, PRE, and PPI at 27-90 g ai/ha in soybeans, POST at 8.8 g ai/ha in peanuts, and POST at 17.5-35 g ai/ha in non-crop land (fence rows, roadsides, equipment storage areas, etc.) It controls many annual broadleaf weeds including cocklebur, jimsonweed, morningglory spp., ragweed spp., redroot pigweed, and smartweed spp. A nonionic surfactant or oil adjuvant is required for maximum foliar activity emerged weeds.

USE PRECAUTIONS

Fire hazard: Technical and the product CLASSIC are dry and non-flammable.
Corrosiveness: Technical chlorimuron and the product CLASSIC are non-corrosive.
Storage stability: Technical chlorimuron and the product CLASSIC are stable if stored free of moisture and high humidity.
Cleaning glassware/spray equipment: NA
Emergency exposure: If ingested, induce vomiting.
Incompatibilities: No physical incompatibilities. May antagonize grass control by POST grass herbicides. The product CLASSIC efficacy may be decreased by tank mixing with contact herbicides.
Spray tank cleanout: Chlorimuron-ethyl, like most other commonly used herbicides must be thoroughly cleaned from the spray tank after each use. First, drain the tank, lines and booms and flush with clean water. Rinse all contaminated surfaces thoroughly. Fill the tank with clean water and add household ammonia at a rate of one gallon of 3% active for every 100 gallons of water. Flush ammonia solution through the lines, booms and nozzles. Turn off the boom and top off the tank and circulate solution for 15 minutes. Flush hoses, boom and nozzles and drain the tank. Remove and clean nozzles, screens and strainers in a bucket of fresh cleaning solution. Repeat the operation. Drain tank and flush system with clean water several times.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 1)
Symptomology: Susceptible plants rapidly stop growing following POST application. Leaves begin to appear chlorotic in 3-5 d, followed by necrosis of the growing point. Complete foliar necrosis and plant death generally occurs 7-21 d after POST application. Some moderately susceptible species remain green but are stunted and usually are out-competed by the crop.
Absorption/translocation: Absorbed readily into leaves and is thoroughly systemic after absorption by roots and foliage.
Metabolism in plants: Metabolic half-life is 1-3 h in tolerant soybeans but >30 h in susceptible cocklebur and redroot pigweed. Soybeans metabolize chlorimuron-ethyl primarily by homo-glutathione conjugation at the 4-chloro group on the pyrimidine ring. A minor metabolite in soybeans is the deesterified chlorimuron acid.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: The mechanism of resistance of most sulfonylurea biotypes is an altered herbicide binding site in the ALS target enzyme or metabolic inactivation.

BEHAVIOR IN SOIL

Sorption: Chlorimuron-ethyl is more tightly adsorbed in the neutral form at low pH values than in the anionic form at high pH values. At lower pHs, chlorimuron-ethyl is more highly adsorbed to OM than to clay.

K_{oc}: Average is 110 mL/g at pH 7 (2)

Transformation:

Photodegradation: Negligible losses

Other degradation: Microbial degradation is fairly slow at all soil pH values. Non-microbial hydrolysis cleaves chlorimuron at the sulfonlurea bridge, releasing CO_2 and producing the aryl sulfonyl amine and the pyrimidinyl amine metabolites. Hydrolysis is slow at high pH when chlorimuron is largely dissociated and negatively charge and is more rapid at lower pH when the molecule is largely neutral.

Persistence: Chlorimuron-ethyl persists longer in high pH soils. Average field half-life is 40 d (2).

Mobility: Mobility or movement in soils is determined by the amount of herbicide adsorbed to the soil. Chlorimuron-ethyl sorption is dependent on soil pH and organic matter content. Chlorimuron-ethyl is less mobile in low pH soils where more herbicide is in the neutral form.

Volatilization: Negligible losses in the field

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade chlorimuron-ethyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 4102 mg/kg; female rat, 4236 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.6 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

CLASSIC: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic Toxicity:

90-d dietary, mouse: NOEL 25 mg/kg

90-d dietary, rat: NOEL male 100 mg/kg**90-d dietary, dog:** NOEL 100 mg/kg

Chronic toxicity:

18-month mouse: NOEL male 1250 mg/kg (highest level tested); not oncogenic

24-month rat: NOEL 250 mg/kg not oncogenic; body and organ weight effects

12-month dog: NOEL 250 mg/kg liver, hemolytic effects at 1500 mg/kg

Teratogenicity:

Rat: NOEL 30 mg/kg/d; not teratogenic; maternal and female toxicity at ≥ 150 mg/kg

Rabbit: NOEL maternal 60 mg/kg/d, fetal 15 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 250 mg/kg in a 2- generation study; maternal and fetal body weight effects

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: In vivo cytogenetics, negative, CHO, negative

DNA damage/repair: In vivo UDS, negative

Wildlife:

Mallard duck oral LD_{50}, >2510 mg/kg; Daphnia 48-h LD_{50}, 1000 mg/L; Bluegill sunfish 48-h LD_{50}, >100 mg/L; Rainbow trout 96-h LD_{50}, >1000 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Product and residue analysis by HPLC

Historical: First synthesized in January 1982 by DuPont with initial field testing in the U.S. and Brazil in 1982. Experimental use permits were granted in 1984 and 1985, and U.S. registration was obtained in 1986. Chlorimuron was first sold commercially in 1986 as CLASSIC.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

chlorotoluron

CAS #: 15545-48-9 $7^{(C_2)}$

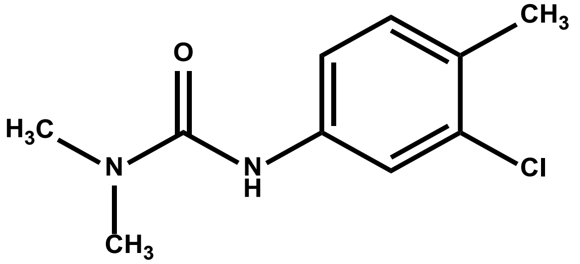
N′-(3-chloro-4-methylphenyl)-*N,N*-dimethylurea

NOMENCLATURE

Common name: chlorotoluron (ANSI, BSI, ISO, WSSA)
Other name(s): 3-(3-chloro-p-tolyl)-1,1-dimethylurea (IUPAC)
Trade name(s): SHUAT; TOLURGAN; TOLUREX; DICURAN®
Chemical family: phenylurea; substituted urea; urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
chlorotoluron



Molecular formula: $C_{10}H_{13}ClN_2O$
Molecular weight: 212.68 g/mole
Description: White powder
Density: 1.4 g/mole (20 C)
Melting point: 148.1 C
Boiling point: NA
Vapor pressure: 1.7×10^{-5} Pa (25 C)
Stability: Stable to heat and UV light; slowly hydrolyzed by strong acids and alkalis
Solubility:
water 74 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 54 ethanol 48
hexane 0.06
pK$_a$: None (non-ionizable)
K$_{ow}$: 2.5 (25 C)

HERBICIDAL USE

Chlorotoluron is a soil-active herbicide and a contact foliar-spray to control many broadleaf and grass weeds on winter cereals, especially against Alopecurus myosuroides.

USE PRECAUTIONS

Fire hazard: Technical and all formulated products are non-flammable.
Corrosiveness: Technical and all formulated products are non-corrosive.
Storage stability: Stable for >1 yr at room temperature
Cleaning glassware/spray equipment: NA
Emergency exposure: Induce vomiting if ingested and seek medical attention; flush eyes with water; wash skin with soap and water; see a doctor if eye or
skin irritation persists; no antidote is known
Incompatibilities: Compatible with hard water

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Interveinal chlorosis of leaf and stem tissue becomes apparent as susceptible seedlings emerge from soil
Absorption/translocation: Absorbed readily into roots by diffusion and translocated acropetally predominately in the xylem
Metabolism in plants: N-dealkylation along with oxidation of the ring-methyl group is the main routes of degradation in plants
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: Stable to ultraviolet light
Other degradation: N-dealkylation and oxidation of the ring methyl group occurs in soil, but N-dealkylation predominates
Persistence: DT$_{50}$ in soil 30 – 40 d
Mobility: NA
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade chlorotoluron unless otherwise indicated.

Acute toxicity:
Oral LD$_{50}$ rat, 9000 mg/kg; Dermal LD$_{50}$ rabbit, >20,000 mg/kg; 4-h inhalation LC$_{50}$, NA; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none
Subchronic toxicity:
90-d dietary, rat: NOEL male 21 mg/kg/d; increased thyroid size
90-d dietary, dog: NOEL 12.7 mg/kg/d; emesis, soft stools
Chronic toxicity:
24-mo dietary, mouse: NOEL 41 mg/kg/d; liver hyperplasia/hypertrophy, hepatoma
24-mo dietary, rat: NOEL 19 mg/kg/d; accelerated aging changes
12-mo dietary, dog: NOEL 1.6 mg/kg/d
6-mo dietary, dog: NOEL 3.75 mg/kg/d; increased liver weight; increased colloidal vacuole in thyroid
Teratogenicity:
Rat: NOEL 400 mg/kg/d; reduced maternal weight gain**Rabbit:** NOEL 10 mg/kg/d; maternal weight decreased; delayed skeletal development

Reproduction:
Rat: NOEL 75 mg/kg/d; increased liver weight in pups.
Mutagenicity:
Gene mutation: Ames test, negative
Structural chromosomal aberration: Negative
DNA damage/repair: UDS, negative
Wildlife:
Bobwhite quail oral LD_{50}, >1250 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Honey bee oral LD_{50}, 235 µg/bee, topical LD_{50}, >236 µg/bee; Daphnia 48-h LC_{50}, >15 mg/L; Bluegill sunfish 96-h LC_{50}, 16.3 mg/L; Rainbow trout 96-h LC_{50}, 8.1 mg/L
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection (who no longer sell or manufacture it)

chlorsulfuron

CAS #: 64902-72-3 **$2^{(B)}$**

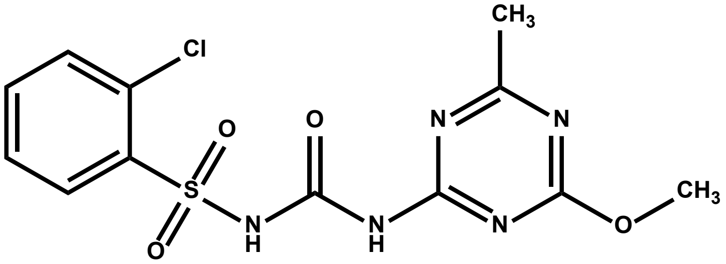
2-chloro-N-[[[4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino] carbonyl]benzenesulfonamide

NOMENCLATURE

Common name: chlorsulfuron (ANSI, BSI, ISO, WSSA)
Other name(s): DPX-W4189; 1-(2-chlorophenylsulf-ony)-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)urea (IUPAC)
Trade name(s): GLEAN®; TELAR®; FINESSE®
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
chlorsulfuron



Molecular formula: $C_{12}H_{12}ClN_5O_4S$
Molecular weight: 357.77 g/mole
Description: White crystalline solid, odorless
Density: NA
Melting point: 174-178 C
Boiling point: NA
Vapor pressure: 3.9×10^{-9} Pa (25 C); Henry's law constant, 3.4×10^{-16} atm m^3/mole
Stability: Slowly degraded by light; decomposes at 192 C
Solubility:
water (25 C), 587 mg/L (pH 5); 31,800 mg/L (pH 7)
organic solvents g/100 mL (25 C):
acetone 5.7
n-hexane <0.001
methanol 1.4
methylene chloride 10.2
toluene 0.3
pK_a: 3.6 (25 C)
K_{ow}: 2.13 (pH 5); 0.10 (pH 7); 0.004 (pH 9)

HERBICIDAL USE

Chlorsulfuron can be applied PRE or POST at 8.8-17.5 g ai/ha in wheat, barely, and oats, PRE at 8.8-17.5 g ai/ha in fallow (preceding wheat), and as a soil or foliar treatment at 13.1-52.6 g ai/ha in non-crop land. Chlorsulfuron controls many broadleaf weeds including kochia, Russian thistle, mustard spp., pigweed spp., and lambsquarters.

USE PRECAUTIONS

Fire hazard: The products GLEAN and TELAR are dry and non-flammable.
Corrosiveness: The products GLEAN and TELAR are non-corrosive.

Storage stability: The products GLEAN and TELAR are stable if stored free of moisture and high humidity.
Cleaning glassware/spray equipment: Wash glassware with detergent and water, and then rinse with acetone. Wash equipment with water and 0.5% v/v chlorine bleach. Rinse several times.
Emergency exposure: May irritate eyes, nose, throat, and skin
Incompatibilities: Compatible with most broadleaf herbicides and fungicides. Do not use spray additives that lower spray pH below 3. Crop injury can occur when mixing with highly acidic liquid fertilizers or surfactants containing liquid fertilizer. Chlorsulfuron applied as a tank mix with certain organophosphate insecticides application can injure small grains, particularly when the crop is stressed.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth of treated plants is inhibited within a few h after application, but injury symptoms usually appear 1-2 wk later. Meristematic areas gradually become chlorotic and necrotic, followed by general foliar chlorosis and necrosis.
Absorption/translocation: Rapid foliar and root absorption. Chlorsulfuron translocates readily in the xylem following root absorption, but less so in the phloem after foliar application. It accumulates in meristematic areas.
Metabolism in plants: Tolerant wheat rapidly hydroxylates chlorsulfuron at the #5 carbon of the phenyl ring, apparently via cytochrome P450 monooxygenases. Hydrolxylated chlorsulfuron then is rapidly conjugated with glucose. Susceptible broadleaves such as soybeans and sugarbeets metabolize chlorsulfuron slowly. Tolerant broadleaves such as flax and black nightshade hydroxylate the methyl group on the triazine ring; followed by rapid glucose conjugation.
Non-herbicidal biological properties: None known.
Mechanism of resistance in weeds: Sulfonylurea-resistant weed biotypes have been selected in the field by chlorsulfuron use. The most common mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: Chlorsulfuron has a more moderate affinity for OM, adsorption to clay is slow.
K_{oc}: Average is 40 mL/g at pH 7 (2) **K_d:** 0.69 mL/g for a Flanagan silt loam
Transformation:
Photodegradation: Negligible under field conditions. Half-life is 1 mo in water under artificial light; stable under artificial light as a dry film on a glass plate; decomposed 30% on dry plant tissue and 15% on dry soil after 1 mo under artificial light
Other degradation: Microbial breakdown is somewhat

slow. Non-microbial hydrolysis plays an important role in chlorsulfuron breakdown, but rates are slow at pH 7.5-8 and increase as pH decreases. Hydrolysis cleaves the sulfonylurea bridge.

Persistence: Average field half-life is 40 d (2), mostly ranging from 4-6 wk. Half-life is shorter at lower pH. Chlorsulfuron residues may injure susceptible crops such as sugarbeets up to 3 or 4 yr after application in high ph soils.

Mobility: Moderately mobile at high pH. Leaching is less at pH <6

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade chlorsulfuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 5545 mg/kg; female rat, 6293 mg/kg; Dermal LD_{50} rabbit, 3400 mg/kg; 4-h inhalation LC_{50} rat, >5.9 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

GLEAN: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic Toxicity:

90-d dietary, mouse: NOEL 2500 mg/kg

90-d dietary, rat: NOEL 100 mg/kg

90-d dietary, dog: NOEL 2500 mg/kg

Chronic toxicity:

24-month mouse: NOEL 500 mg/kg; not oncogenic; body weight effects at 5000 mg/kg

24-month rat: NOEL 100 mg/kg not oncogenic; body weight effects at 500 mg/kg

12-month dog: NOEL 2000 mg/kg; slight body weight and hematological effects at 7500 mg/kg

Teratogenicity:Rat: NOEL 165 mg/kg/d; not teratogenic; maternal at 500 mg/kg/d, and fetal toxicity at ≥1500 mg/kg/d

Rabbit: NOEL 200 mg/kg/d not teratogenic; maternal toxicity at 400 mg/kg/d, and fetal toxicity at >1000 mg/kg/d

Reproduction:

Rat: NOEL 500 mg/kg; toxic effects at 2500 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: Rat dominant lethal, negative; in vitro test, negative

DNA damage/repair: Rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >1000 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck, oral LD_{50}, >1000 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Earthworm, LC_{50} in soil, >2000 mg/kg; Honey bee, LD_{50}, >25 µg/bee; Daphnia 48-h LC_{50}, 370 mg/L; Bluegill sunfish 96-h LC_{50}, >250 mg/L; Rainbow trout 96-h LC_{50}, >250mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Product analysis by HPLC; residue determined by HPLC and by immunoassay

Historical: Introduced by Du Pont. Chlorsulfuron was the first commercialized sulfonylurea in the U.S.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

cinmethylin

CAS # Isomeric mixture: 87818-31-3

30$^{(R)}$

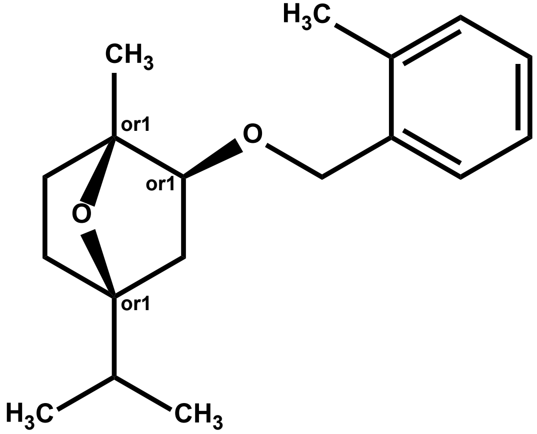
(1R,2S,4S)-rel-1-methyl-4-(1-methylethyl)-2-[(2-methylphenyl)methoxy]-7-oxabicyclo[2.2.1]heptane

NOMENCLATURE

Common name: cinmethylin (ANSI, BSI, ISO, WSSA)
Other name(s): cinmethyline; SD 95481; (1*RS*, 2*SR*,4*SR*)-1,4-epoxy-*p*-menth-2-yl-2-methylbenzyl ether (IUPAC)
Trade name(s): ARGOLD®
Chemical family: None generally accepted

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
cinmethylin



Molecular formula: $C_{18}H_{26}O_2$
Molecular weight: 274.40 g/mole
Description: Amber liquid
Density: 1.01 g/mL (20 C)
Melting point: NA
Boiling point: 313 ± (2 C) (1.013×10^5 Pa)
Vapor pressure: 1.02×10^{-2} Pa (20 C)
Stability: Degraded by light in the presence of air; Hydrolytically stable at pH 3-11 (25 C); <5% decomposition after 30 d
Solubility:
water 63 ± 5 mg/L (20 C)
pK_a: None (non-ionizable)
K_{ow}: 6850 ± 360

HERBICIDAL USE

Cinmethylin can be applied at 0.025-0.1 kg ai/ha in transplanted rice. It also can be applied PPI or PRE at 0.56-1.7 kg ai/ha in soybeans, cotton, and peanuts, as well as certain broadleaf vegetables, trees, vines, and ornamentals. Cinmethylin primarily controls annual grasses, but also controls certain annual broadleaf weeds and sedges. It has no U.S. registration, but is registered in various countries outside the U.S.

USE PRECAUTIONS

Fire hazard: Technical is non-flammable
Corrosiveness: Technical is non-corrosive to mild steel
Storage stability: Technical is stable for >2 yr
Cleaning glassware/spray equipment: Wash or flush with water.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood. Cinmethylin disrupts meristematic development in roots and shoots. (more details see page 16)
Symptomology: NA
Absorption/translocation: Absorbed through the shoots and roots of germinating or emerging weeds, followed by upward translocation in the xylem.
Metabolism in plants: Metabolized by plants to a complex series of hydroxylation and oxidation products, most of which become conjugated.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed by soil
K_{oc}: Average is 300 mL/g (1)
Transformation:
Photodegradation: Rapidly photodegraded in natural sunlight
Other degradation: Readily metabolized in soil with CO_2 as the major terminal degradation product
Persistence: Under aerobic conditions, field half-life ranges from 25-78 d, increasing with higher OM content. Under anaerobic conditions (e.g. flooded rice paddy), the degradation rate is reduced because of slower microbial degradation.
Mobility: Limited mobility in soil
Volatilization: Minimal losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cinmethylin unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 4553 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, mild
Subchronic toxicity: NA
Chronic toxicity:
18-mo dietary, mouse: NOEL 30 mg/kg
24-mo dietary, rat: NOEL 100 mg/kg
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife:
Bobwhite quail oral LD_{50}, >2150 mg/kg; Mallard duck oral LD_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, 7.2 mg/L; Bluegill sunfish 96-h LC_{50}, 6.4 mg/L; Rainbow trout 96-h LC_{50}, 6.6 mg/L

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA

Historical: First reported in 1985 (2). Introduced by Shell International Chemical Company Ltd. in China in 1989. Cinmethylin never was registered in the U.S. and was discontinued by Du Pont around 1990. It was registered in Japan in 1994.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF
Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Way, J. W. et al. 1985. Proc. Br. Crop Prot. Conf.-Weeds 1:265.

cinosulfuron

CAS #: 64593-91-6

2(B)

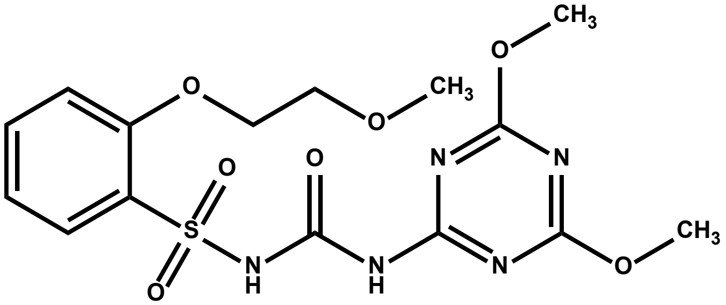
N-[[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]carbonyl]-2-(2-methoxyethoxy)benzenesulfonamide

NOMENCLATURE

Common name: cinosulfuron (ISO approved)
Other name(s): CGA 142464; 1-(4,6-dimethoxy-1,3,5-triazin-2-yl)-3[2-(2-methoxyethoxy)phenylsulfonyl]urea (IUPAC)
Trade name(s): SETOFF
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
cinosulfuron



Molecular formula: $C_{15}H_{19}N_5O_7S$
Molecular weight: 413.41 g/mole
Description: Colorless crystalline powder
Density: 1.47 g/mL (20 C)
Melting point: 127.0-135.2 C
Boiling point: NA
Vapor pressure: <1 x 10^{-5} Pa (25 C)
Stability: Decomposes above the melting point. No significant hydrolysis at pH 7-10; considerable hydrolysis at pH 3-5
Solubility:
water (25 C), 120 mg/L (pH 5); 4000 mg/L (pH 6.7); 19000 mg/L (pH 8.1)
acetone, 36000 mg/L ethanol, 1900 mg/L
toluene 540 mg/L (25 C)
pK_a: 4.72 (weak acid)
K_{ow}: log K_{ow} = 2.04 (pH 2.1, 25 C)

HERBICIDAL USE

Cinosulfuron is sulfonylurea herbicide for POST control of grass and broadleaf weeds such as water plantain, nutsedge, water clover, pondweed, pickerel weed and gooseweed in transplanted, direct seeded, and wet/water/dry seeded flooded rice crops at 60-80 g ai/ha.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: NA
Storage stability: NA
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth of susceptible plants is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by slow, general foliar chlorosis and necrosis.
Absorption/translocation: Moves in both the xylem and phloem
Metabolism in plants: Cinosulfuron is metabolized in paddy rice primarily via cleavage of the sulfonylurea linkage followed by *O*-demethylation of the ethoxymethoxy substituent. Aryl hydroxylation of parent cinosulfuon has been observed to occur.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 20 mL/g
Transformation: Cinosulfuron is primarily decomposed by hydrolysis of the sulfonylurea linkage.
Persistence: DT_{50} in soils under laboratory and field conditions were 20 and 3 d, respectively.
Mobility: May be leachable
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cinosulfuron unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg, 4-h inhalation LC_{50} rat, >5 mg/L (max. attainable conc.); Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none
Chronic toxicity:
12-mo dietary, dog: NOEL 2500 mg/kg, not oncogenic
24-mo dietary, rats: NOEL 400 mg/kg
Wildlife:
Japanese quail oral LD_{50}, >2000 mg/kg; Honey bee LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >2500 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA

Analytical methods: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Roberts, T. 1998. Metabolic Pathways of Agrochemicals.

clethodim

CAS #: 99129-21-2

1$^{(A)}$

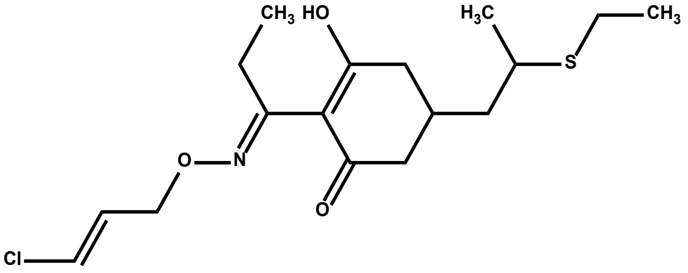
2-[(1E)-1-[[[(2E)-3-chloro-2-propenyl]oxy]imino]propyl]-5-[2-(ethylthio)propyl]-3-hydroxy-2-cyclohexen-1-one

NOMENCLATURE

Common name: clethodim (ANSI, BSI, ISO, WSSA)
Other name(s): clethodime; cletodim; cletodin; RE-45601; (E)-2-[1-[[(3-chloro-2-propenyl)oxy]imino] propyl]-5-[2-(ethylthio)propyl]-3-hydroxy-2-cyclohexen-1-one; (E) (±)-2-[1-[[(3-chloro-2-propenyl)oxy]imino]propyl]-5-[2-(ethylthio)propyl]-3-hydroxy-2-cyclohexen-1-one; (5RS)-2-{(E)-1-[(2E)-3-chloroallyloxyimino]propyl}-5-[(2RS)-2-(ethylthio) propyl]-3-hydroxycyclohex-2-en-1-one (IUPAC)
Trade name(s): SELECT®; PRISM®; ARROW®; OSPRAY®; SEGARD®; ENVOY®
Chemical family: cyclohexanedione; cyclohexane-dione oxime; cyclohexenone; cyclohexene oxime

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
clethodim



Molecular formula: $C_{17}H_{26}ClNO_3S$
Molecular weight: 359.91 g/mole
Description: Clear, amber, viscous liquid
Density: 1.40 g/mL (20 C)
Melting point: NA
Boiling point: NA
Vapor pressure: <1.33 x 10^{-5} Pa (20 C)
Stability: Unstable at extreme pHs and temperatures; degraded by UV light
Solubility: NA

pK_a: 4.1 (weak acid) **K_{ow}:** 0.49 (pH 9); 40 (pH 7)

>3,000 (pH 5)

HERBICIDE USE

Clethodim can be applied POST at 0.11- 0.28 kg ai/ha) in cotton and soybeans for control of many annual and perennial grasses. An oil adjuvant is needed for maximum efficacy. Clethodim has no activity against broadleaf weeds and sedges.

USE PRECAUTIONS

Fire hazard: Product is non-flammable; flash point is (110 C)
Corrosiveness: NA
Storage stability: <1 and <3% degradation in glass and aluminum containers, respectively, after 1 yr of storage at 21 C.
Cleaning glassware/spray equipment: Wash glassware with detergent and rinse. A commercial tank cleaner may be used for removing residues from a spray tank.

Emergency exposure: Wash skin with soap and water. Flush eyes with water for at least 15 min. If ingested, drink water or milk and contact a physician; do not induce vomiting unless directed to do so by medical personnel. Typical signs of toxicity observed in lab animals include salivation, decreased motor activity, unsteady gait, and hyperactivity.
Incompatibilities: Grass control by clethodim may be antagonized when tank mixing with bentazon and, to a lesser extent, with acifluorfen.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)
Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop within 1-3 wk of application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.
Absorption/translocation: Clethodim penetrates the cuticle within 1 h of application and subsequent rainfall does not reduce its activity (3). Little information is available on clethodim translocation. Presumably, it translocates similar to sethoxydim which is primarily moved in the symplasm (including the phloem) with eventual accumulation at the growing points.
Metabolism in plants: Soybeans, cotton, and lettuce metabolize clethodim to a major and a minor metabolite, both of which are conjugates. Residue levels decline during growth of the plant. Clethodim is rapidly photodecomposed on leaf surfaces by an acid-catalyzed reaction. Adjuvants increased the rate of clethodim photodegradation on leaves (1).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Most weed biotypes that have developed resistance to aryloxyphenoxy propionates with cross-resistance to the cyclohexandeiones appear to have an ACCase that is insensitive to the herbicide. However, in diclofop-resistant rigid ryegrass from Australia, cross-resistance to a number of herbicides including sethoxydim is not due to differential ACCase sensitivity (4). Rather, resistance may be due to increased herbicide metabolism or by sequestration away from the site of action.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil
K_d: 0.05-0.23 mL/g (five soils)
Transformation:
Photodegradation: Half-life was 1.7 d on a sandy loam

in natural sunlight, producing the sulfoxide; half-life in the dark, however, was 2 d, indicating that photodegradation rate is significant, but may be unimportant given the extremely rapid rate of non-photodegradative processes.

Other degradation: Hydrolysis half-lives (25 C) were 28 d (pH 5), 300 d (pH 7), and 310 d (pH 9) C. Major products result from: 1) interconversion between the E and Z geometric isomers about the C = N oxime double bond and 2) degradation to an oxazole and E-1-chloropropen-3-ol.

Persistance: Non-persistent in soil with a half-life of ~3 d

Mobility: NA

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade clethodim unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 1630 mg/kg, female rat, >1360 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >3.9 mg/L; Skin irritation,rabbit, none; Skin sensitization, NA; Eye irritation, NA

SELECT 2EC: Oral LD_{50} male rat, 3610 mg/kg; female rat, 2920 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >4.4 mg/L; Skin irritation rabbit, moderate; Skin sensitization, guinea pig, no; Eye irritation rabbit, corneal involvement or irritation clearing in 8-21 d

Subchronic toxicity:

90-d dietary, mouse, rat and dog: NOEL NA, decreased body weight; increased liver size and anemia

21 d-dermal, rat: Systemic NOEL 50 mg/kg/d; LOEL 10 me/kg/d

Chronic toxicity:

18-mo dietary, mouse: Systemic NOEL male 200 mg/kg, female 1000 mg/kg; LOEL male 200 mg/kg, female 1000 mg/kg; Tests done with 83.3% technical

24-mo dietary, rat: Systemic NOEL 19 mg/kg/d (500 mg/kg); systemic LOEL 100 mg/kg/d (2500 mg/kg); no effects; tests done with 83% technical

12-mo dietary, dog: NOEL 1 mg/kg/d; systemic LOEL 75 mg/kg/d; increased absolute and relative liver weights; alternations in hematology and clinical chemistry; Tests done with 83.3% technical

Teratogenicity:

Rat: Study 1 with 82.6% technical: NOEL 100 mg/kg/d; LOEL 350 mg/kg/d; reduced body weight gain and clinical signs of toxicity in mother; skeletal anomalies and reduced body weight in fetus; not teratogenic. Study 2 with 98.6% technical: NOEL maternal 10 mg/kg/d, NOEL fetal 100 mg/kg/d; LOEL maternal 100 mg/kg/d, LOEL fetal 700 mg/kg/d; significant reductions in fetal body weight and litter size; increased litter and fetal incidence of cervical rib at 700 mg/kg/d; not teratogenic

Reproduction:

Rat: Systemic NOEL 51 mg/kg/d (500 mg/kg); systemic LOEL 263 mg/kg/d (2500 mg/kg); reduced body weight, particularly in males, and decreased food consumption in both generations; no other effects; tests done with 83.3% technical grade

Mutagenicity:

Gene mutation: Ames test, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2000 mg/kg; 8-d dietary LC_{50}, >4370 mg/L; Mallard duck 8-d dietary LC_{50}, >3978 mg/L; Honey bee oral LD_{50}, >100 µg/bee; bluegill sunfish 96-h LC_{50}, 33 mg/L; rainbow trout 96-h LC_{50}, 18 mg/L

SELECT 2EC: Honey bee oral LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 20.2 mg/L\

Use classification: General Uses

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: HPLC with UV detection at 254 nm can be used with linearity between 80 and 200 µg/mL. A Shandon ODS-Hypersil (or other C-18) column of 5 µm in pore size, 4.6 mm i.d., and 25 cm length is used. Isocratic eluant is 68.6% acetonitrile/1.4% acetic acid/30% water and flow rate is 1 mL/min.

MANUFACTURER(S) AND INFORMATION SOURCES

Industry source(s): Valent; Micro Flo; Adama

Reference(s):

1. Falb, L. N. et al. 1990 J. Agric. Food Chem. 38:875.
2. Focke and Lichtenthaler. 1987. Z. Naturforsch. 42c:1361.
3. Kincade, R. T. Et al. 1987. Proc. Br. Crop Prot. Conf. Weeds. 1:49.
4. Powles, S. B. et al. 1990. Pages 394-406 in M. B. Green, H. M. LeBaron, and W. K. Moberg, eds., Managing Resistance to Agrochemicals. Am. Chem. Soc. Symp. Ser. 421, Washington DC.
5. Rendina and Felts. 1988. Plant Physicol. 86: 983.
6. Ashworth, D. J. 1988. Clethodim Technical Product Chemistry: Series 63 (Study No. 8828545). Chevron Chemical Company. Richmond, CA.

clodinafop-propargyl

CAS #: 105512-06-

1(A)

2-propynyl(2R)-2-[4-[(5-chloro-3-fluoro-2-pyridinyl)oxy]phenoxy]propanoate

NOMENCLATURE

Common name: clodinafop-propargyl

Other name(s): CGA-184927; prop-2-ynyl(R(-2-[4-(5-chloro-3-fluoro-2-pryridyloxy)phenoxy]propionate (IUPAC)

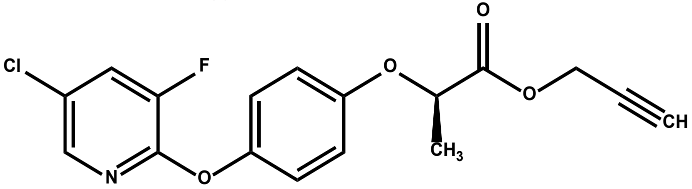
Trade name(s): DISCOVER™

Chemical family: aryloxyphenoxy propionic acid; aryloxyphenoxy propionate; pyridylphenylether; oxyphenoxy acid ester

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

clodinafop-propargyl



Molecular formula: $C_{17}H_{13}ClFNO_4$

Molecular weight: 349.8 g/mole

Description: Cream colored, odorless, fine powder

Density: 1.37 g/mL (22 C)

Melting point: 48.2 – 57.1 C

Boiling point: NA

Vapor pressure: 3.2 x 10^{-6} Pa (25 C)

Stability: Stable at room temperature

Solubility:

water 4.0 mg/L (pH 7, 25 C)

organic solvents g/L (25 C)

acetone	880
n-octanol	25
ethanol	97
toluene	690
n-hexane	8.6

pK_a: 2.91 (clodinafop acid) (weak acid)

K_{ow}: log K_{ow} = 3.9

HERBICIDE USE

Clodinafop-propargyl is a broad spectrum graminicide with activity on many annual and perennial grass species. When used with the cloquintocet-mexyl safener, it can be applied POST at 40 to 80 g ai/ha on all types of wheat with excellent crop tolerance. Barley is not completely safened by cloquintocet-mexyl. Clodinafop-propargyl controls many common grass weeds of wheat including: wild oats, canarygrass, green, yellow, and giant foxtails, Persian darnel, barnyardgrass, and annual ryegrass. Crop oil concentrate is required for maximum POST efficacy.

USE PRECAUTIONS

Fire hazard: Technical clodinafop-propargyl is a solid and non-flammable. Formulated products are liquids with a flash point of 61.7 C (NFPA Class IIIA Combustible Liquid).

Corrosiveness: Formulated products are non-corrosive.

Storage stability: Formulated product can be safely stored at freezing temperatures. Return to original state by warming at room temperature and agitating prior to use.

Cleaning glassware/spray equipment: Clean glassware and spray equipment with 1% solution (v/v) of household ammonia. In spray equipment use a pressure rinser to direct the ammonia solution inside the tank. Clean nozzles and screens separately.

Emergency exposure: If ingested, do not induce vomiting. Induction of emesis is not recommended due to the large amount of petroleum solvent in this product, which could cause chemical pneumonitis if aspirated. If ingested, lavage stomach, taking care to avoid aspiration of stomach contents into the lungs.

Incompatibilities: Formulated clodinafop-propargyl mixes with a wide range of pesticide tank-mix partners and can be applied with liquid nitrogen fertilizer consisting of up to 50% of the spray carrier.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)

Symptomology: Growth of susceptible weeds is inhibited within 48 h after application. The leaves of susceptible weeds turn yellow, red, or brown after several days, followed by death of the growing point. Complete weed death occurs 1 to 3 weeks after application, depending on weed species and growing conditions. Weeds not completely killed by clodinafop-propargyl are often stunted and are less completitive with the crops.

Adsorption/translocation: Both clodinafop-propargyl and cloquintocet-mexyl are rapidly taken up by plant foliage. Warm, humid conditions favor uptake. The addition of crop oil concentrate improves leaf penetration, especially under dry conditions. Formulated product is generally rainfast in 30 min. Translocation in grasses is predominately by the phloem; rapid with accumulation in the meristematic tissues. Higher temperatures and relative humidities result in faster translocation in the plant.

Metabolism in plants: Clodinafop-propargyl is rapidly metabolized in wheat, and the metabolites that form exist primarily as sugar conjugates. Cleavage of the ester to form the free acid is the major initial step. The free acid is further metabolized by hydroxylation adjacent to the pyridinyl nitrogen to form (R)-2-[4-[(6-hydroxy-5-chloro-3-fluoro-2-pyridinyloxy)phenoxyl] propanoic acid. Further metabolism from the free acid involves cleavage of the pyridinyloxy-phenoxy ether bridge to form (R)-2-(4-hydroxyphenoxy) propanoic acid and 5-chloro-3fluoro-2(1H)pyridinone. This pyridinyl-specific metabolite undergoes further metabolic transformations, and a portion is incorporated into natural products such as glucose. A minor metabolic route is cleavage of the phenoxy-propanoic acid ether bridge to form (R)-4-[(5-chloro-3-fluoro-2-pyridinyl)oxy phenol.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: ACCase inhibitor-resistant weed biotypes selected in the field by other ACCase inhibitor herbicides are often, but not always resistant to clodinafop-propargyl. Resistance can be due to altered ACCase binding site or enhance metabolism.

BEHAVIOR IN SOIL

Sorption: Medium to slight

K_{oc} and K_d values: median K_{oc} was 1588 mL/g. Adsorption K_{oc} = 251 mL/g and K_d = 2.42 mL/g for loamy sand pH 7.2, 0.96% OC; K_{oc} = 1829 mL/g and K_d = 12.8 mL/g for a sand pH 6.7, 0.7% OC; K_{oc} = 1195 mL/g and K_d =16.6 mL/g for a silt loam pH 6.5, 1.4% OC; K_{oc} 2364 mL/g and K_d = 99.3 mL/g for a silt loam pH 7.1, 4.2% OC; K_{oc} = 1588 mL/g and K_d = 311.3 mL/g for a muck soil pH 6.7, 19.6% OC. This indicates that clodinafop-paropargyl has a low potential of mobility in the soil profile.

Transformation:

Photodegradation: The photolytic half-life in water was 11 h; photolysis on wet viable silty loam soil was 0.8 h and 318 h on dry sterile soil.

Other degradation: Chemical degradation proceeds through the conversion of the ester to the acid to biologically non-active compounds; under aerobic soil metabolism conditions the half-life of the parent ranged from 0.5 to 2 d and the acid approximately 5 to 20 d; conversion to CO_2 occurs very fast indicating rapid mineralization by soil microorganisms; aerobic aquatic and anaerobic aquatic half-lives of clodinafop-propargyl were <1 d. Hydrolysis occurred faster at pH 9 ($t_{1/2}$ = 2.2 h), compared to pH 7 ($t_{1/2}$ = 64 h) and pH 5 ($t_{1/2}$ = 184 d).

Persistence: Clodinafop-propargyl dissipated rapidly under soil and climatic conditions of the western Canadian prairies, with a $t_{1/2}$ <1 d.

Mobility: The parent herbicide has a leaching index of 3 indicating a low leaching potential. The acid derivatives of both the herbicide and the safener can be classified as being moderately mobile in the soil. However, due to their low solubility in water their fast degradation pattern and the low use rates involved, their potential for leaching is also extremely low. Clodinafop-propargyl remained in the top 10 cm of soil in field studies conducted under soil and climatic conditions of the western Canadian prairies.

Volatilization: Negligible losses from treated plants, soil and water

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade clodinafop-paropargyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1829 mg/kg; Dermal LD_{50}, >2000 mg/kg; Acute inhalation LC_{50} (rat), >2.33 g/L (the highest attainable concentration); Eye irritation rat, slightly irritating; Skin irritation rat, minimally irritating; Skin sensitization guinea pig, positive

DISCOVER 2EC: Oral LD_{50} (rate – males, females), 2231 mg/kg, 2240 mg/kg (respectively); Dermal LD_{50} (rat – both species), >4000 mg/kg; Acute inhalation LC_{50} (rat), >3.5 mg/L; Eye irritation, severely irritating; Skin irritation moderately irritating; Skin sensitization, positive to guinea pig.

Subchronic toxicity:

90-d dietary, rat: NOEL 0.93 mg/kg (15 ppm)

90-d dietary, dog: NOEL 0.36 mg/kg (10 ppm)

Chronic toxicity:

18-m dietary, mouse: NOEL 1.1 mg/kg (10 ppm)

24-m dietary, rat: NOEL 0.32 mg/kg (10 ppm)

12-m dietary, dog: NOEL 3.4 mg/kg (100 ppm)

Teratogenicity:

Rat: NOEL maternal and fetal, 40 mg/kg/d; not teratogenic

Rabbit: NOEL maternal, 25 mg/kg/d; fetal, 125 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 3.2 mg/kg/d (50 ppm); no reproductive effects at up to 1000 mg/kg for two generations

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Human lymphocytes, negative; Mouse micronucleus, negative

DNA damage/repair: Rat hepatocytes, negative; Human fibroblasts, negative

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: A multi-step process culminating with the coupling of a functionalized propionic acid with a halogenated pyridine followed by esterification with propargyl alcohol

Purification of technical: Crystallized from industrial methylated spirits containing 6% water

Analytical methods: Percentage active ingredient in clodinafop-propargyl technical is determined by wide-bore capillary gas chromatography with OV-1701 as the stationary phase and using methyl isobutyl ketone as the diluting solvent

Historical: Clodinafop- propargyl was discovered by Ciba-Geigy Ltd. with first patents received in 1982 and first registration in Switzerland in 1991. It has since been registered in over 30 countries including Canada in 1994 and the U.S. in 2000.

MANUFACTURER(S) AND INFORMATION SOURCES

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Amreim J., Nyffeler A., and Rufener J., CGA 184927 + Safener: A new postemergence grasskiller for use in small grain cereals. Brighton Crop Protection Conference-Weeds, 1989, Vol 1, pp 71-76.
2. Cornes, D.W., Scott D., Henderson E.J., and Ryan P.J., The efficacy and crop safety of a herbicide + safener combination in cereals under UK conditions. Brighton Crop Protection Conference-Weeds, 1989, Vol 2, pp 729-734.
3. Holm F.A., Kirkland K.J., and Stevenson F.C.,

Defining optimum herbicide rates and timing for wild oat (Avena fatua) control in spring wheat (Triticum aestivum). Weed Technology, 2000, Vol 14, pp 167-175.

4. Kreuz K., Gaudin J., Stingelin J., and Ebert E., Mode of action of the new herbicide safener CGA 185072 in wheat. International Conference on Herbicide Safeners, 1990, Budapest Hungary.
5. Kreuz K, Gaudin J., Stingelin J., and Ebert E., Metabolism of the aryloxyphenoxy-propanoate herbicide, CGA-184927, in wheat, barley and maize – differential effects of the safener, CGA-185072. Z. Naturfrosch. 1991, 46c, 901-905.

clomazone

CAS #: 81777-89-1

$13^{(F_3)}$

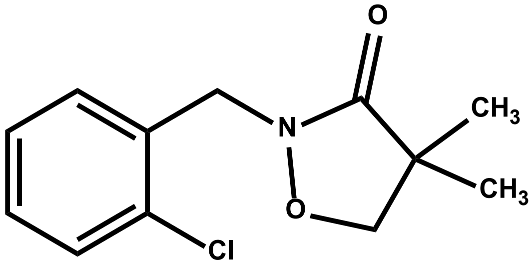
2-[(2-chlorophenyl)methyl]-4,4-dimethyl-3-isoxazolidinone

NOMENCLATURE

Common name: clomazone (ANSI, BSI, ISO, WSSA).
Other name(s): dimethazone (discontinued common name); fenoxan; FMC 57020; 2-(2-chlorobenzyl)-4,4-dimethyl-1,2-oxazolidin-3-one (IUPAC); 2-(2-chlorobenzyl)-4,4-dimethylisoxazolidin-3-one (IUPAC)
Trade name(s): COMMAND®; CENTIUM®
Chemical family: isoxazolidinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
clomazone



Molecular formula: $C_{12}H_{14}ClN_2$
Molecular weight: 239.70 g/mole
Description: Colorless to pale yellow, viscous liquid at room temperature, White, crystalline solid below the melting point.
Density: 1.19 g/mL (20 C)
Melting point: 25 C
Boiling point: 275.4 C (1.013 x 10^{-5} Pa)
Vapor pressure: 1.92 x 10^{-2} Pa (25 C)
Stability: Relatively stable to UV light (slowly degraded by sunlight in aqueous solution, but sensitizers such as acetone greatly enhance the degradation rate); decomposes at >200 C; not hydrolyzed in aqueous solution buffered at a range of pH values (acidic, neutral, basic)
Solubility:
water 1100 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone soluble
acetonitrile soluble
chloroform soluble
cyclohexanone soluble
oil (refined) 90
dioxane soluble
heptane soluble
dimethy formamide soluble
methylene chloride soluble
n-hexane soluble
kerosene 4.5-5
methanol soluble
soybeans
toluene soluble
xylene soluble
pK_a: None (non-ionizable)
K_{ow}: 350

HERBICIDAL USE

Clomazone can be applied PRE or PPI at 0.56-1.4 kg ai/ha in soybean and cotton; applied PPI, PRE, or POST-Transplant 0.84-1.12 kg ai/ha in tobacco; applied PPI at 0.56-1.12 kg ai/ha in pepper; applied PRE or PPI up to 1.12 kg ai/ha in pumpkin; applied PRE at 0.45-0.67 kg ai/ha in rice; applied PRE to layby at 1.12-1.4 kg ai/ha in sugarcane. Clomazone products are also registered for use on a wide range of vegetable crops under various state registrations. Clomazone controls a wide spectrum of annual broadleaf and grass weeds including velvetleaf, common ragweed, common lambsquarters, barnyardgrass, *Panicum* spp., and crabgrasses. Clomazone can be impregnated on dry bulk fertilizer or applied by a conventional sprayer.

USE PRECAUTIONS

Fire hazard: Clomazone technical is non-flammable; flash point is 157 C (setaflash closed cup). COMMAND 4 EC and COMMANDE 3ME are non-flammable; flash points are 40 C and >94 C, respectively.
Corrosiveness: COMMAND 4 EC and COMMAND 3 ME are non-corrosive.
Storage stability: Shelf life of COMMAND 4 EC and COMMAND 3ME is >2 yr. COMMAND 4 EC and COMMAND 3ME should be stored above 4.4 C and 20 C respectively. Freezing temperatures crystallize the active ingredient within COMMAND 4 EC, but crystals can be re-dissolved with >15.5 C and shaking.
Cleaning glassware/spray equipment: Wash with detergent and water.
Emergency exposure: Wash skin with soap and water. Flush eyes with water and seek immediate medical attention. If ingested, rinse mouth with water and dilute by drinking 1-2 glasses of water; do not induce vomiting.
Incompatibilities: Compatible with water of ≤1000 mg/L hardness and with most herbicides and liquid fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Recent evidence suggests that clomazone is metabolized to its 5-keto form which is the active form. The 5-keto form inhibits 1-deoxy-D-xyulose 5-phosphate synthase (DOXP), a key component to plastid isoprenoid synthesis. (more details see page 14)
Symptomology: Susceptible seedlings usually emerge from treated soil, but are bleached white and become necrotic after several days. Susceptible species in later growth stages may exhibit foliar bleaching when treated POST or when exposed to clomazone vapor drifting from nearby treated areas.
Absorption/translocation: Not highly absorbed when foliar-applied. Clomazone is readily absorbed by roots and emerging shoots (grass coleoptile and broadleaf hypoocotyl), and is translocated in the xylem to the folage. Clomazone appears to translocate poorly in the phloem.
Metabolism in plants: Oxidative cleavage, yielding metabolites with greater polarity, was the primary detoxification reaction in soybeans and velvetleaf (7).

Differences in metabolism among species did not correlate with relative susceptibility (4,5).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 300 mL/g (6)

Transformation:

Photodegradation: Slowly degraded in aqueous solution exposed to sunlight. Clomazone loss from soil by photolysis is lower than that by microbial degradation

Other degradation: Readily degraded by microbes under aerobic conditions. Aerobic degradation proceeds by oxidative mechanisms resulting in CO_2 evolution and formation of bound residues. Rate and extent of aerobic degradation varies with soil characteristics. Clomazone degradation is faster under flooded (anaerobic) than aerobic conditions. Anaerobic decomposition proceeds primarily by reductive ring opening. Non-microbial hydrolysis of clomazone apparently does not occur.

Persistence: Average field half-life is 24 d (6), but varies with soil characteristics. Half-lives were about 16 d in sandy loam and 36 d in silt loam soils. Increasing soil pH from 5.5 to 6.5 with lime decreases persistence. Clomazone persistence is lower in sandy loam than in silt loam or clay loam soils.

Mobility: In laboratory studies, clomazone has low mobility in most soils, but moderate mobility in fine sand. A soil degradate formed under anaerobic conditions has greater mobility than parent clomazone in all soils studied. In 60-d field test, clomazone remained in the top 30 cm of a loamy sand with 1.2% OM receiving high amounts of water.

Volatilization: Losses can occur from moist soil surfaces.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade clomazone unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 2077 mg/kg; female rat, 1369 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} male rat, 6.52 mg/L, female rat, 4.23 mg/L; Skin irritation rabbit, minimal; Skin sensitization guinea pig, no; Eye irritation rabbit, practically none

COMMAND 4 EC: Oral LD_{50} male rat, 2343 mg/kg; female rat, 1406 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 4.59 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

COMMAND 3ME: Oral LD_{50} female rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; Acute inhalation LC_{50} rat, 5.21 mg/L; Skin irritation rabbit, non-irritating; Eye irritation rabbit, non-irritating

Subchronic toxicity:

90-d dietary, mouse: NOEL 1000 mg/kg; not carcinogenic

90-d dietary, rat: NOEL 1000 mg/kg; not carcinogenic

Chronic toxicity:

18-mo dietary, mouse: NOEL 1000 mg/kg; not carcinogenic

24-mo dietary rat: NOEL 1000 mg/kg; not carcinogenic

12-mo dietary, dog: NOEL 500 mg/kg

Teratogenicity:

Rat: NOEL 100 mg/kg/d; not teratogenic at ≤600 mg/kg/d

Rabbit: NOEL 30 mg/kg/d; not teratogenic at ≤700 mg/kg/d

Reproduction:

Rat: NOEL 1000 mg/kg in a 2-generation study; not a reproductive toxin at ≥4000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative with or without metabolic activation

Structural chromosome aberration: Rat *in vivo* cytogenetics, negative

DNA damage/repair: Primary culture rat hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, ≥2510 mg/kg; dietary LC_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg; dietary LC_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, 5.2 mg/L; Atlantic silverside 96-h LC_{50}, 6.26 mg/L; Bluegill sunfish 96-h LC_{50}, 34 mg/L, NOEC 8.9 mg/L; Rainbow trout 96-h LC_{50}, 19 mg/L, NOEC 8.9 mg/L; Sheepshead minnow 96-h LC_{50}, 5.2 mg/L; Mysid shrimp 96-h LC_{50}, 0.566 mg/L

Use classification: General use, EPA Class IV

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React *N*-(2-chlorophenylmethyl)hydro-xylamine with chloropivaloyl chloride, followed by ring closure with methanolic KOH.

Purification of technical: Recrystallization from organic solvents, or distillation.

Analytical methods: Reverse phase HPLC under temperature control is used for analysis of technical and formulated products. GC may be used for analysis of formulated products and is used with N-P detection or GC-MS detection for analysis of resides.

Historical: Clomazone was developed in the early 1980s and commercialized as COMMAND in 1985. It is protected under U.S. patent 4,405,357. Numerous foreign patents also have been assigned.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): FMC; Helena

Reference(s):

1. Croteau, R. 1992. Plant Physiol. 98:1515.
2. Devine, M., S.O. Duke, and C. Fedtke. 1991. Physiology of Herbicide Action. Prentice Hall, New Jersery.
3. Duke, S.O. et al. 1991. Weed Sci. 39:339.
4. Liebl and Norman. 1991. Weed Sci. 39:329.
5. Scott and Weston. 1992. Weed Sci. 40:7.
6. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
7. Weimer, M. R. et atl. 1992. Pestic. Biochem. Physiol. 42:43. (comment: not enough space?)
8. Weimer, M. R. et al. 1992. Plant Physiol. 98:427.
9. Ferhatoglu, Y., M. Barret, and J. Chappell. 2002. Abstracts. WSSA 42:73.

clopyralid

3,6-dichloro-2-pyridinecarboxylic acid

CAS # Acid: 1702-17-6
Methyl: 1532-24-7
Monoethanol amine: 57754-85-5
Potassium: 58509-83-4

$4^{(O)}$

NOMENCLATURE

Common name: clopyralid (ANSI, BSI, WSSA)

Other name(s): 3,6-DCP; DOWCO 290; Acid dichloro-3,6 picolinique; 3,6-dichloropicolinic acid (IUPAC); 3,6-dichloropyridine-2-carboxylic acid (IUPAC)

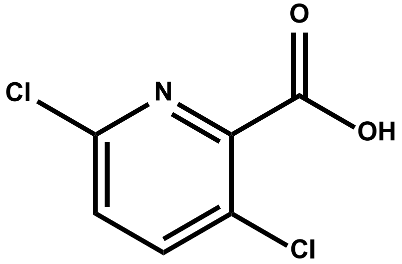
Trade name(s): ACCENT GOLD®; BATTLESHIP®; COLT® AS; CONFRONT®; CURTAIL®; CURTAIL® M; HORNET® WDG; LONTREL® TURF AND ORNAMENTAL; MILLENNIUM ULTRA®, RECLAIM®; REDEEM® R&P; STINGER®; TRANSLINE®; WIDEMATCH®

Chemical family: picolinic acid; pyridinecarboxylic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure(s):

clopyralid acid



Molecular formula: *Acid* $C_6H_3Cl_2NO_2$; *Monoethanolamine (Mea) salt* $C_8H_{10}Cl_2N_2O_3$; *Methyl* $C_7H_5Cl_2NO_2$; *Potassium* $C_6H_2Cl_2KNO_2$

Molecular weight: *Acid* 192.00 g/mole; *Methyl* 206.03 g/mole; *Mea salt* 253.08 g/mole; *Potassium* 230.09 g/mole

Description: Off-white crystalline solid, odorless

Density: 0.30 g/mL

Melting point: 151-152 C

Boiling point: NA

Vapor pressure: 1.36×10^{-3} Pa (25 C)

Stability: Unstable in acid, oxidizing material, and halogenated organics; stable to UV light; decomposes above 151 C

Solubility:

Acid
water 1000 mg/L (25 C)
organic solvents g/100 mL (25 C):
octanol 13.9
hexane 0.50
xylene 0.65

Monoethanolamine salt
water 300,000 mg/L (25 C) (7)

pK_a: 2.3 (weak acid)

K_{ow}: $\log K_{ow} = -1.81$ (pH 5); -2.63 (pH 7); -2.55 (pH 9)

HERBICIDAL USE

Clopyralid can be applied postemergence at 0.105-0.28 kg ae/ha in sugarbeets, Christmas trees (conifers), grasses for seed, fallow, field corn, and to labeled fruits and vegetables at variable labeled rates as well as at 0.14-0.56 kg ae/ha in pasture, rangeland, and on Conservation Reserve land. Clopyralid controls many annual and perennial broadleaf weeds including Canada thistle, wild buckwheat, cocklebur, jimsonweed, ragweed spp., marshelder, and wild sunflower.

USE PRECAUTIONS

Fire hazard: STINGER, TRANSLINE, and RECLAIM are combustible; flash point is 47 C. CONFRONT is combustible; flash point is 66 C. CURTAIL is noncombustible; flash point is >91 C.

Corrosiveness: STINGER, TRANSLINE, RECLAIM, and CONFRONT corrode brass, copper, zinc, and aluminum. CURTAIL corrodes brass and copper.

Storage stability: Stable for 2 yr. Store CONFRONT, RECLAIM, STINGER, and TRANSLINE above -2.2 C or warm to 4.4 C and agitate before use. Store CURTAIL above -12 C or warm and agitate before use.

Cleaning glassware/spray equipment: Rinse and flush equipment at least three times with water; add household ammonia at 1% v/v during the second rinse.

Emergency exposure: Wash skin with soap and water. Wash eyes with water or injury may result.

Call a poison control center or doctor immediately for treatment advice.

Incompatibilities: All formulated products are compatible with most types of hard water.

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood but similar to that of endogenous auxin (IAA) and other auxin-type herbicides (more details on page 14)

Symptomology: Symptoms are typical of other auxin-type herbicides, and include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. At low concentrations, the tips of young leaves may develop narrow feather-like extensions of the midrib.

Absorption: Readily absorbed by roots and foliage. In sunflower and rapeseed, 97% of foliar-applied clopyralid was absorbed within 24 h of application (2). Clopyralid parent acid is more rapidly absorbed than either the ester or salt forms. Under conditions of low humidity or water stress, absorption of the monoethanolamine and K salts are greatly reduced, whereas the acid and ester forms are unaffected. Uptake of clopyralid across plant membranes occurs by diffusion of the parent acid, and presumably leads to accumulation of clopyralid in cells due to ion trapping that is common with most weak acid herbicides.

Translocation: Readily transported in plant tissues, primarily via the symplasm (including the phloem). Over 50% of applied clopyralid translocated out of the treated leaves of Canada thistle within 24 h of application (3). Clopyralid accumulates at the growing points. Salt forms of clopyralid translocate less than the parent acid, but twice as much as the esters (1). This appears to result from increased partitioning of clopyralid esters in the cuticle.

Metabolism in plants: Slowly metabolized in most plants. In Canada thistle, no clopyralid metabolites were found 9 d after treatment in one study, whereas 22% of the herbicide was present as water-soluble metabolites 6 d after application in another study (2, 6). Rapeseed rapidly metabolized clopyralid, with 38 and 70% converted to water-soluble metabolites 1 and 6 d after treatment, respectively (6).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed. Clopyralid is dissociated and negatively charged in soil because of its low pKa.

K_{oc}: Average is 6 mL/g (7), but ranges to 60 mL/g (increased soil sorption with time).

Transformation:

Photodegradation: Negligible losses

Other degradation: Degraded by microbes; non-microbial degradation does not occur

Persistence: Moderate residual with an average field half-life of 40 d (7). Half-life was 12-70 days across a range of U.S. soils. Soil residues may injure certain crops (such as peas, lentils, and potatoes), a crop rotation interval of 18-months is typical for susceptible crops.

Mobility: Moderate leaching potential

Volatilization: Insignificant losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade clopyralid acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, mouse, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >1.3 mg/L; Skin irritation rabbit, none or very slight; Skin sensitization guinea pig, no; Eye irritation rabbit, severe (possible corneal injury and permanent vision impairment)

Subchronic toxicity:

90-d dietary, mouse: NOEL 750 mg/kg/d

90-d dietary, rat: NOEL 300 mg/kg/d

90-d dietary, dog: NOEL 150 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 500 mg/kg/d; not oncogenic

24-mo dietary, rat: NOEL 50 mg/kg/d; not oncogenic

12-mo dietary, dog: NOEL 100 mg/kg/d

Teratogenicity:

Rat: NOEL >250 mg/kg/d; not teratogenic

Rabbit: NOEL 110 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 500 mg/kg/d; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: Mouse bone marrow, negative

DNA damage/repair: Rat UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, 1465 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; long-term reproductive NOEL, 1000 mg/kg; Earthworm LC_{50} in soil, 1000 mg/kg; Honey bee oral LD_{50}, 100 μg/bee, topical LD_{50}, >100 μg/bee; Daphnia 48-h LC_{50}, >99.0 mg/L; 21-d NOEC, 17 mg/L; Bluegill sunfish 96-h LC_{50}, >102 mg/L; Rainbow trout 96-h LC_{50}, >99.9 mg/L; Fathead minnow ELS NOEC, 10.8 mg/L*;* green algae 96-h E_bC_{50}, 32.7 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: See reference 4

Historical: Clopyralid was discovered in 1961. The original patent has expired. Clopyralid was first marketed in 1978 in Europe. In the U.S., CURTAIL was introduced in 1987, STINGER in 1988, and CONFRONT in 1989.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences;

Reference(s):

1. Bovey, R. W. et al. 1989. Weed Sci. 37:19.
2. Hall and Vanden Born. 1988. Weed Sci. 36:9.
3. O'Sullivan and Kossatz. 1984. Weed Res. 24:17.
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5. Thomson and Cobb. 1987. Proc. Br. Crop Prot. Conf.-Weeds 3:1097.
6. Turnbull and Stephenson. 1985. Weed Sci. 33:143.
7. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
8. Syracuse Environmental Research Associates, Inc. 2004. Clopyralid Human health and ecological risk assessment - Final Report. SERA TR 04-43-17-03c. Report dated December 5, 2004. Available at: http://www.fs.fed.us/foresthealth/pesticide/pdfs/120504_clopyralid.pdf

cloquintocet-mexyl

CAS #: 99607-70-2

NC

1-methylhexyl [(5-chloro-8-quinolinyl)oxy]acetate

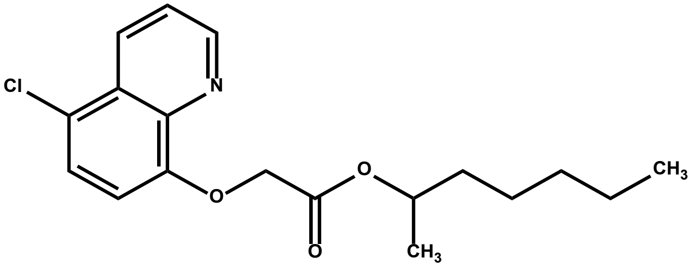
NOMENCLATURE

Common name: cloquintocet-mexyl (ISO)
Other name(s): CGA-185072 (code name); (*RS*)-1-methylhexyl (5-chloroquinolin-8-yloxy)acetate (IUPAC)
Trade name(s): DISCOVER^{TM}; HORIZON; TOPIK; AXIAL
Chemical family: quinolynoxyacetate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

cloquintocet-mexyl



Molecular formula: $C_{18}H_{22}C1NO_3$
Molecular weight: 335.83 g/mole
Description: Colorless crystalline solid
Density: NA
Melting point: 69 C
Boiling point: NA
Vapor pressure: 2.5 x 10^{-6} Pa (20 C)
4.6 x 10^{-2} Pa (30 C); 1.6 x 10^{-1} Pa (40 C)
Stability: Stable
Solubility:
water 0.8 mg/L (20 C)
organic solvents g/100 mL (20 C):
acetone >50
dichloromethane >50
ethyl acetate >50
hexane 0.75
methanol 18
octanol 21
toluene >50**pK_a**: 3.1 (weak acid)(cloquintocet acid)
K_{ow}: log K_{ow} = 5.1 (RP-TLC-method)

HERBICIDAL USE

Cloquintocet-mexyl is a herbicide safener protecting wheat, rye and triticale against injury from the aryloxyphenoxypropionate herbicides clodinafop-propargyl and pinoxaden. Cloquintocet-mexyl protects barley only partially. The formulated tank mixture of the herbicide and safener (4:1 ratio, v/v) is applied POST for the control of annual grass weeds in wheat. It is registered for use in Europe (1), United States and Canada.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent.
Emergency exposure: If on skin, wash with plenty of soap and water. Get medical attention if irritation persists. If in eyes, flush with plenty of water. Call a physician if irritation persists. If inhaled, remove victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Cloquintocet-mexyl accelerates the initial metabolism of the herbicide clodinafop-propargyl in wheat, which proceeds via hydroxylation and ether cleavage (2). The subsequent conjugation of the hydroxylated herbicide with glucose is also accelerated by the safener in wheat (2). The safener was less effective in enhancing the metabolism of the herbicide clodinafop-propargyl in barley and corn (2).
Symptomology: No symptoms are visible, since the compound is not phytotoxic.
Absorption/translocation: The formulated mixture of the herbicide and safener is applied postemergence to the leaves of wheat and the other protected cereal crops. Cloquintocet-mexyl is generally absorbed rapidly by wheat leaves (2).
Metabolism in plants: NA
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: None known

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: NA
Other degradation: NA
Persistence: NA
Mobility: NA
Volatilization: Non-volatile
Formulation effects: Environmental fate properties are unaffected by formulation type.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cloquintocet-mexyl unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >2000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, >935 mg/L; Primary eye irritation rabbit, non-irritant; Skin irritation rabbit, negative
Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife: NA
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Synthesis during manufacturing results in technical active ingredient with a purity >99%. No additional purification is needed.

Analytical methods: Chromatographic methods (TLC, GC, and HPLC) are available. Contact Syngenta Crop Protection for details.

Historical: This safener was introduced by Ciba-Geigy in 1989. It is used in combination with clodinafop-propargyl and pinoxaden world wide.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Amhrein A. et al. 1989. Proc. Brighton Crop Prot. Conf.-Weeds, pp. 71-76.
2. Kreuz, K. et al. 1990. Z. Naturforsch. 46c:901.

cloransulam-methyl

CAS #: 147150-35-4 **2$^{(B)}$**

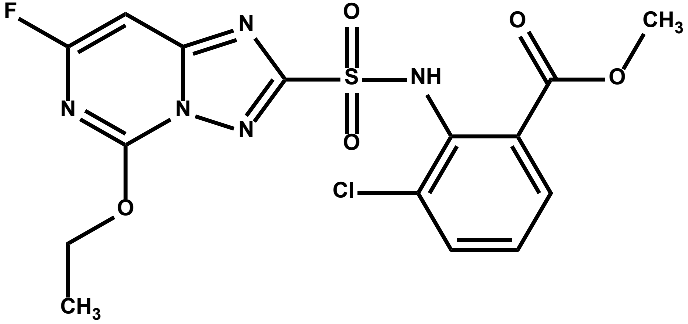
methyl 3-chloro-2-[[(5-ethoxy-7-fluoro[1,2,4]triazolo[1,5-*c*] pyrimidin-2-yl)sulfonyl]amino]benzoate

NOMENCLATURE

Common name: cloransulam-methyl (ANSI, ISO, WSSA)
Other name(s): XDE-565 (code number); methyl 3-chlor-2-(5-ethoxy-7-fluoro[1,2,4]triazolo[1,5-c]pyrimidin-2-ylsulfonamido)benzoate (IUPAC); methyl 3-chloro-N-(5-ethoxy-7-fluoro[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)sulfonyl] amino]benzoate (IUPAC)
Trade name(s): AMPLIFY®; AUTHORITY™ FIRST DF; FIRSTRATE®; FRONTROW®; GANGSTER™; SONIC™
Chemical family: sulfonanilide; triazolopyrimidine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
cloransulam-methyl



Molecular formula: $C_{15}H_{13}ClFN_5O_5S$
Molecular weight: 430 g/mole
Description: Off-white powdered solid
Density: 1.58 g/mL
Melting point: 216-218 C
Boiling point: NA
Vapor pressure: 3.94 x 10^{-14} Pa (25 C)
Stability: Stable after 28 d (50 C)
Solubility:
- water 3 mg/L (pH 3-5, 25 C); 184 mg/L (pH 7, 25 C)
- organic solvents mg/L (25 C)
- acetone 4360
- acetonitrile 5500
- dichloromethane 6980
- ethyl acetate 980
- methanol 470
- octanol 10

pK_a: 4.81 (weak acid)

K_{ow}: 1.12 (pH 5)

HERBICIDAL USE

Cloransulam-methyl is used for control of many key broadleaf weeds in soybeans. The product FIRSTRATE is used in conventional, minimum-till, or no-till soybeans soil-applied at rates of 35 to 44 g ai/ha or POST at 17.5 g ai/ha or 35 g ai/ha for heavy weed infestations or added residual control. FIRSTRATE is applied burndown surface preplant, PPI, or PRE for the control of cocklebur, horseweed (marestial), mallow, smartweed, velvetleaf, morningglory, giant and common ragweed sunflower, pigweed, jimsonweed, and lambsquarters. Soil applications of FIRSTRATE in combination with a grass herbicide provide broad spectrum control. FIRSTRATE can also be used POST for the control of many key broadleaf weeds such as cocklebur, velvetleaf, marestail, morningglory, giant, and common ragweed, sunflower, jimsonweed, and sicklepod among others. FIRSTRATE is applied POST with adjuvant systems including nonionic sufcatant, crop oil concentrate or methylated seed oil. FIRSTRATE can be used POST in combination with many other POST herbicides for the control of grasses or other broadleaves.

USE PRECAUTIONS

Fire hazard: The product FIRSTRATE is dry and non-combustible.
Corrosiveness: Does not react with mild steel or stainless steel at 50 C
Storage stability: FIRSTRATE has no storage temperature restrictions and is stable up to 2 years on the shelf.
Cleaning glassware/spray equipment: Clean with water of alkaline cleaner such as ammonia.
Emergency exposure: Wash skin with soap and water. If ingested, induce vomiting immediately as directed by medical personnel.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Most sensitive weed species are killed before emergence following soil application of chloransulam-methyl, but weeds may die after emergence under some conditions. Emerged sensitive species exhibit stunting, growing point effects, interveinal discoloration (purpling) and necrosis within 1-3 weeks. Following POST applications, initial symptoms occur within 3-10 days. These include stunting, growing point inhibition, and chlorosis followed by necrosis. Complete death of susceptible weeds occurs within 2-3 weeks.
Absorption/translocation: Soil applied cloransulam-methyl is absorbed primarily by the roots, with some absorption by emerging shoots. Cloransulam-methyl is readily translocated from roots to shoots and from shoots to roots.
Metabolism in plants: The initial metabolism of cloransulam-methyl in soybeans is displacement of fluorine with homoglutathione. The reaction is catalyzed by a homogluthathione S-transferase enzyme (hGST). The half-life in tolerant soybeans is 5 h, while the half-lives in susceptible velvetleaf, pitted morningglory, and ivyleaf morningglory were 62, 69, and 165 d, respectively.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Numerous weed species (including prickly lettuce, kochia, Russian thistle, cocklebur, ragweed, and pigweeds and others) have been reported to have evolved resistance to ALS-type herbicides due to an altered ALS enzyme. Resistant biotypes are naturally occurring and are slightly different in their genetics. In addition, cross-resistance can occur to different classes of ALS-inhibitors.

BEHAVIOR IN SOIL

Sorption: Greater adsorption at low vs. high soil pH. Sorption tends to increase with time associated with the soil.

Aged K_{oc}: Range from 54.4 to 915 mL/g after 3 mo incubation on six different soils

K_d: 0.38 ± 0.26 L/kg.

Transformation:

Photodegradation: The half-life of cloransulam-methyl for aqueous photolysis is 20 min. and for soil photolysis is 13 days.

Other degradation: Cloransulam-methyl degraded microbially in aerobic and anaerobic aquatic systems (half-life 16 d). Cloransulam-methyl also degraded hydrolytically under alkaline conditions with a half-life of 3 days at pH 9.0, greater than 200 days at pH 7 and stable at pH 5. The main pathway of degradation in soil appears to be microbial rather than hydrolytic or photolytic.

Persistence: Residues of cloransulam-methyl reach non-phytotoxic levels within 14 to 33 d. The persistence profile of cloransulam-methyl allows planting of important rotational crops such as corn, cotton, and sorghum within 9 months, and wheat within 6 mo.

Lab experiments: Half-life in different soils ranged from 13 to 28 d

Field studies: Half-life ranging from 8 to 10 d have been indicated in field studies

Mobility: Assessment in the field indicated little movement into the soil profile. Residues were contained in the upper 30 to 45 cm of the soil.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cloransulam-methyl acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >3.77 mg/L; Primary eye irritation rabbit, slight irritant; Skin irritation rabbit, negative; Skin sensitizationguinea pig, none; Neurotoxicity rat >2000 mg/kg

FIRSTRATE formulation: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Primary eye irritation rabbit, none; Skin irritation rabbit, negative; Skin sensitization guinea pig, none

Subchronic toxicity:

90-d dietary, mouse: NOEL male 50 mg/kg/d; female 100 mg/kg/d

90-d dietary, rat: LOAEL < 100 mg/kg/d

90-d dietary, dog: NOAEL 40 mg/kg/d

90-d neurotoxicity, rat: NOAEL 2000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 10 mg/kg/d; not oncogenic

24-mo dietary, rats: NOEL 10 mg/kg/d; not oncogenic

12-mo dietary, dog: NOEL 5 mg/kg/d

Teratogenicity:

Rat: >1000 mg/kg/d (maternal & developmental); not teratogenic

Rabbit: NOEL 100 mg/kg/d (maternal); NOEL 300 mg/kg/d (developmental); Not teratogenic

Reproduction:

Rat: NOEL 100 mg/kg/d (reproductive capability, growth & survival); not reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

DNA damage/repair: Chromosomal aberration assay, negative; Cytogenic assay, negative
in vivo mouse micronucleus, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary oral LC_{50}, >5620 mg/L; Mallard duck, oral LD_{50}, >2000 mg/kg; 8-d dietary oral LC_{50}, >5620 mg/L; Earthworm NOEC in soil, > 2000 mg/kg; Honey bee 48-h acute contact LD_{50}, >25 µg/bee; Daphnia 48-h EC_{50}, >185.3 mg/L; Bluegill sunfish 96-h acute LC_{50}, >154 mg/L; Rainbow trout 96-h LC_{50}, >86 mg/L; Grass shrimp 96-h LC_{50}, >121 mg/L; Eastern oyster 96-h acute EC_{50}, >111 mg/L, NOEC, 111 mg/kg; Green algae EC_{50}, 3.46 mg/L, NOEC, 0.122 mg/L; Blue green algae EC_{50}, 12.4 µg/L, NOEC, 564 µg/L; Freshwater diatom EC_{50}, 1.79 mg/L, NOEC, 0.427 mg/L; Marine diatom EC_{50}, 3.55 mg/L, NOEC, 0.438 mg/L; Duckweed EC_{50}, 2.91 mg/L, NOEC not calculated **Use classification:** General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Contact Dow AgroSciences

Historical: Cloransulam-methyl was discovered in 1989. FIRSTRATE and FRONTROW (cloransulam + flumetsulam) herbicides were both registered on US soybean in 1997.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences; FMC; Valent

copper chelate

copper ethylenediamine or triethanolamine

CAS # Ethylenediamine complex:
13426-91-0
Triethanolamine complex: 31089-39-1

NC

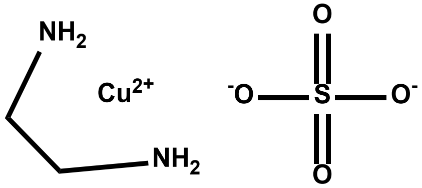
NOMENCLATURE

Common name: copper chelate
Other name(s): ethylenediamine; 1,2-ethanediamine
Trade name(s): AQUATRINE™; CUTRINE® PLUS; CUTRINE-PLUS GRANULAR; STOCKTRINE® II; KOMEEN®; K-POOL™; K-TEA™
Chemical family: None generally recognized

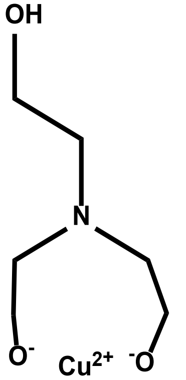
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
Structures for the copper ethylenediamine and triethanolamine complexes are somewhat uncertain.

Copper ethylene diamine



Copper triethanolamine



Molecular formula: *Ethylenediamine complex*: $C_2H_{12}CuN_2O_2$; *Sulfate salt of ethylenediamine complex*: $C_2H_{12}CuN_2O_6S$; *Triethanolamine complex*: $C_6H_{15}CuNO_4$
Molecular weight: *Ethylenediamine complex*: 159.68 g/mole; *Sulfate salt of ethylenediamine complex*: 255.73 g/mole; *Triethanolamine complex*: 228.74 g/mole
Description: Dry technical is not available because the complexes are manufactured from an integrated process beginning with copper sulfate (ethylenediamine) or copper hydrate (triethanolamine). Most subsequent information in this section is provided for formulated products.
Density: *KOMEEN*: 1.22 g/mL; *K-TEA:* 1.20 g/mL
Melting point: *KOMEEN*: NA (loss of water of hydration and decomposition at high temperatures with charring); *K-TEA:* NA (loss of water of hydration and decomposition at high temperatures with charring)
Boiling point: *KOMEEN* (102 C); *K-TEA:* NA
Vapor pressure: Elemental copper and copper ethylenediamine and triethanolamine complexes are nonvolatile.
Stability: Stable to light; unstable below pH 6

Solubility:
KOMEEN
water completely miscible (25 C)
organic solvents (25 C):
benzene immiscible
chloroform immiscible
DMSO miscible
ethanol miscible
isopropanol miscible
kerosene immiscible
methanol miscible
toluene immiscible
methylene chloride immiscible
n-hexane immiscible
K-TEA
water completely miscible (25 C)
organic solvents (25 C):
benzene immiscible
chloroform immiscible
DMSO miscible
ethanol miscible
isopropanol miscible
kerosene immiscible
methanol miscible
toluene immiscible
methylene chloride immiscible
n-hexane immiscible

pK_a: *Triethanolamine complex* 4.23
K_{ow}: NA

HERBICIDAL USE

Copper chelates are used primarily to control algal growth in impounded waters, lakes, ponds, reservoirs, stock tanks, and irrigation conveyance systems. Copper chelates are applied at 0.2-1 mg/L of elemental copper.

USE PRECAUTIONS

Fire hazard: All products are aqueous or dry and noncombustible. Auto-ignition temperature of CUTRINE-PLUS is >96 C.
Corrosiveness: All products are non-corrosive to mild steel, aluminum, and brass.
Storage stability: Indefinite storage life. All products are stable to temperatures below freezing and above 90 C.
Cleaning glassware/spray equipment: Wash with water.
Emergency exposure: Wash skin and eyes with water. If ingested, call a doctor. Symptoms of poisoning include appetite loss and jaundice. Copper accumulates in the liver.
Incompatibilities: Ethanolamine formulations are effective in fresh, salt, and brackish waters but not in water with pH below 5. Water with pH below 6 may destroy the chelating of ethylenediamine and triethanolamine formulations causing copper precipitation. Triethanolamine formulations may become less effective if applied to water cooler than 15.5 C.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. May inhibit photosystem II electron transport.
Symptomology: Cells become chlorotic, turning whitish or brown. Floating mats of algae may fail to sink immediately unless broken up by rain or wind.

Absorption/translocation: Readily absorbed by algal cells, but with little intercellular movement. Uptake by vascular plants varies by species. Copper is translocated throughout vascular aquatic plants and may be stored or excreted.

Metabolism in plants: Elemental copper cannot be metabolized but may bind with proteins within the plant to form complexes that persist in detritus formed from plant decomposition.

Non-herbicidal biological properties: Fungicidal and bactericidal properties in controlling fish and shrimp diseases.

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed by clay and OM

Transformation: Elemental copper cannot be degraded, but the chelating agents probably are microbially degraded

Persistence: Elemental copper persists indefinitely, becoming unavailable in sediment or recycled by aquatic plants as a micronutrient

Mobility: NA

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with formulated products as indicated.

Acute toxicity:

KOMEEN: Oral LD_{50} rat, 498 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 0.81 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

K-TEA: Oral LD_{50} rat, 1312 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 0.54 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity: NA**Chronic toxicity:** NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

CUTRINE-PLUS: Mallard duck 8-d dietary LC_{50}, >1000 mg/kg; Bluegill sunfish 96-h LC_{50}, 1.2 mg/L in soft water, 7.5 mg/L in hard water; Channel catfish 96-h LC_{50}, 6 mg/L; Rainbow trout 96-h LC_{50}, <0.2 mg/L in soft water, 4 mg/L in hard water; Blue shrimp 96-h LC_{50}, 19 mg/L; Grass shrimp 96-h LC_{50}, 4.8 mg/L; Fiddler crab 96-h LC_{50}, 156 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Copper triethanolamine and ethylenediamine complexes are synthesized by reacting a copper compound with triethanolamine or ethylenediamine, respectively.

Purification of technical: NA

Analytical methods: Triethanolamine and ethylenediamine complexes can be determined by neutralization with acetic acid followed by standard iodometric titration.

Historical: Copper ethanolamine complex was first synthesized by Applied Biochemists in 1973 and patented under U.S. patent 3,930,834. Copper ethylenediamine complex was first synthesized by Griffin in 1977 and patented under U.S. patent 4,361,435.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Applied Biochemists; Griffin

copper sulfate

sulfuric acid copper (2+)salt (1:1)

CAS #: 7758-98-

NC

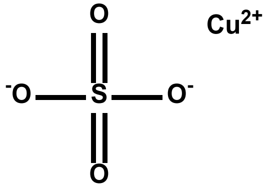
NOMENCLATURE

Common name: copper sulfate
Other name(s): cupric sulfate (IUPAC); copper (2+) tetraoxosulfate (IUPAC); copper(II) tetraoxosulfate (IUPAC)
Trade name(s): COPPER-2; STAR GLOW POWDER; STAR SHINE CRYSTALS; TRIANGLE BRAND COPPER SULFATE CRYSTAL
Chemical family: None generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

copper sulfate



Molecular formula: CuO_4S
Molecular weight: 159.60 g/mole;
Description: Blue tricline crystals
Density: 2.28 g/mL
Melting point: Loses 4 H_2O at 110 C
Boiling point: Decomposes before boiling
pK_a: NA
K_{ow}: NA

HERBICIDAL USE

Copper sulfate is used primarily to control algal growth in impounded waters, lakes, ponds, reservoirs, and irrigation conveyence systems. It is applied at 0.2-1 mg/L of elemental copper, depending on algae species and water hardness. When applied in continuous low doses, pondweed is controlled in irrigation conveyance systems. Copper sulfate can be dissolved in water and sprayed onto the pond or lake surface. Fine crystals can be dusted onto the water surface and large crystals can be placed in a burlap bag and towed behind a boat. In irrigation conveyance systems, large or granular crystals can be dumped into ditches at intervals. For pondweed control, finer crystals can be metered into flowing water. Potable water has a tolerance of 1 mg/L copper.

USE PRECAUTIONS

Fire hazard: All products are aqueous or dry and are non-combustible.
Corrosiveness: Highly corrosive to plain and galvanized steel, but does not corrode stainless steel, monel, or plastic.
Storage stability: Dry products have indefinite storage life if maintained dry and are stable to heat or cold extremes that could occur in facilities lacking temperature control.
Cleaning glassware/spray equipment: Wash and rinse with water.
Emergency exposure: Flush eyes with water for 15 min and get medical attention. If ingested, induce vomiting, and call a physician.
Incompatibilities: Decreased effectiveness with increasing water hardness. Efficacy is significantly reduced when $CaCO_3$ alkalinity exceeds 150 mg/L. Fish toxicity decreases as alkalinity increases.

BEHAVIOR IN PLANTS

Mechanism of action: Low copper levels are needed for plant growth. Excess levels apparently kill algae by causing an imbalance with other enzyme metal cofactors, resulting in enzyme blockage.
Symptomology: Cells become chlorotic, turning white or brown. Floating mats of algae may fail to sink immediately unless broken up by rain or wind.
Absorption/translocation: Readily absorbed by most single-celled, colonial, and filamentous algae. Absorption by the alga species *Chara* may be inhibited by accumulation of calcium carbonate around the plant body. Alternatively, the difficulty in controlling *Chara* with copper may result from copper precipitation in the hard water in which *Chara* grows. Other algae such at *Pithophora* and *Cladophora* also are difficult to control with copper sulfate as copper cannot penetrate the thick mats and binds to the cell walls of these algae. Copper sulfate generally is assumed to be poorly absorbed by most higher plants. Foliar- and soil-absorbed copper is translocated throughout the plant.
Metabolism in plants: Elemental copper cannot be metabolized.
Non-herbicidal biological properties: Fungicidal, bactericidal, and nutritional.
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed by clay and OM. Copper can precipitate on clay particles as copper hydroxides, phosphates, or carbonates.
Transformation: Elemental copper cannot be degraded.
Persistence: Applied elemental copper becomes part of the native copper content of soil.
Mobility: Copper has low leachability in soil due to strong adsorption.
Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade copper sulfate pentahydrate (hydrated form) unless indicated otherwise.
Acute toxicity:

Oral LD_{50} rat, 470 mg/kg; Dermal LD_{50} rabbit, >8000 mg/kg; 4-h inhalation LC_{50} rat, >1.48 mg/L; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation rabbit, corrosive

Subchronic toxicity: NA

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Pheasant oral LD_{50}, 1000 mg/L (estimated); Bluegill sunfish 96-h LC_{50}, 44 mg/L (0.884 mg Cu/L) in soft water at 18 C; 7.3 mg Cu/L in hard water; Rainbow trout 96-h LC_{50}, 0.135 mg Cu/L soft water (13 C); Blue crab 96-h LC_{50}, 28 mg Cu/L; Shrimp 96-h LC_{50}, 17 mg Cu/L; Oyster 96-h LC_{50}, 5.8 mg Cu/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: $Cu + O_2 + H_2SO_4 \rightarrow CuSO_4 \cdot 5H_2O$

Purification of technical: Crystallization from water

Analytical methods: Electrolytic deposition and wet chemical analysis using KI titrated with $Na_2S_2O_3$.

Historical: Used for algae control in the U.S. since about 1905.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Boliden Intertrade;
Griffin; Helena; Phelps Dodge

cyanazine

CAS #: 21725-46-2 **$5^{(C_1)}$**

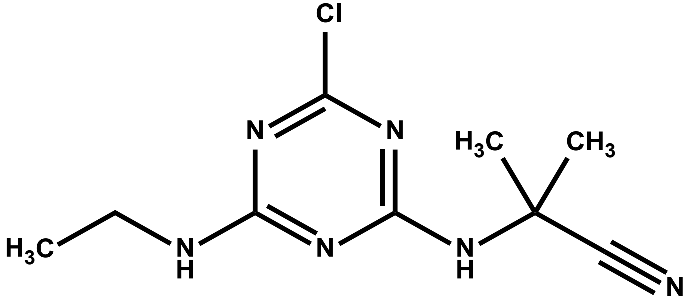
2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile

NOMENCLATURE

Common name: cyanazine (BSI, ISO, WSSA)
Other name(s): SD 15418; WL 19805; 2-chloro-4-(1-cyano-1-methylethylamino)-6-ethylamino-1,3,5-triazine; 2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methylpropiononitrile (IUPAC); 2-[[4-chloro-6-(ethylamino)-*s*-triazin-2-yl]amino]-2-methylpropiononitrile
Trade name(s): BLADEX®; EXTRAZINE®; CYPRO
Chemical family: chloro-*s*-triazine; chlorotriazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
cyanazine



Molecular formula: $C_9H_{13}ClN_6$
Molecular weight: 240.70 g/mole
Description: Colorless crystals
Density: 0.35 g/mL fluffed; 0.45 g/mL packed
Melting point: 167.5-169 C
Boiling point: NA
Vapor pressure: 2.1 x 10^{-7} Pa (20 C); 1.3 x 10^{-6} Pa (30 C); 7.8 x 10^{-6} Pa (40 C)
Stability: Stable to heat and UV light; stable between pH 5 and 9; hydrolyzed by strong acid and base
Solubility:
water 160 mg/L (23 C), 171 mg/L (25 C)
organic solvents g/100 mL (20 C):acetone 19.5 acetonitrile soluble ethanol 4.5
benzene 1.5 ethyl acetate soluble
carbon tetrachloride <1 *n*-hexane ≤ 0.02
chlorobenzene <10 methylcyclohexanone 21
chloroform 21
methylene chloride soluble
dichloromethane 14.5 xylene <10
pK_a: 1.6 (weak base)
K_{ow}: 127

HERBICIDAL USE

Cyanazine can be applied as follows: early preplant, PPI, PRE, or POST at 0.9-5.3 kg ai/ha in corn; PPI or PRE at 0.9-4 kg ai/ha in sweet corn; and early preplant, PRE, and directed-POST at 0.6-1.3 kg ai/ha in cotton. Additional uses outside the U.S. include PRE at 0.8-2.2 kg ai/ha in peas, POST at 0.2-0.4 kg ai/ha in cereals, and PRE at 1-2 kg ai/ha in field beans.
Cyanazine controls many annual broadleaf weeds, including morningglory spp., purslane, common ragweed, wild mustard, and kochia, and several grass species such as foxtail spp., witchgrass, crabgrass spp., and barnyardgrass. A surfactant or oil adjuvant may improve efficacy with POST applications.

USE PRECAUTIONS

Fire hazard: Formulated products are non-flammable
Corrosiveness: Formulated products are non-corrosive
Storage stability: Shelf lives of liquid BLADEX and EXTRAZINE products are 2 yr
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: Wash skin with water. Flush eyes with water; call a physician if irritation persists. If ingested, drink 1-2 glasses of water and induce vomiting; call a physician.
Incompatibilities: Compatible with most pesticides and liquid fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Interveinal or marginal chlorosis of leaves followed by necrosis (browning) beginning at the leaf margins and progressing toward the center; symptoms are observed first on lower leaves when soil-applied
Absorption/translocation: Readily absorbed by foliage or roots. Use of an oil adjuvant increases foliar uptake. Leaf-absorbed cyanazine may concentrate somewhat along leaf margins but little moves out of the treated leaves. Root-absorbed cyanazine moves readily up to the shoots via the xylem. Root uptake following POST applications enhances weed control.
Metabolism in plants: Root-applied cyanazine is rapidly converted to hydroxy-cyanazine in corn roots with benzoxazinone as catalyst. Corn roots and shoots appear to oxidize the nitrile group at significant rates but dealkylate the cyanazine molecule slowly. Rates of glutathione conjugation and benzoxazinone-catalyzed hydroxylation appear to be slow in corn shoots.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Over 60 species worldwide have developed triazine-resistant biotypes. Those studied at the genetic level have an altered *psbA* gene coding for a glycine in place of a serine on the D1 protein on which the cyanazine binding site is located. Thus, triazines cannot bind efficiently to the D1 protein and do not block photosynthetic electron transport.

BEHAVIOR IN SOIL

Sorption: Reversibly adsorbed to soil particles. Adsorption increases with increased OM, lower pH, and lower soil water content.

K_{oc}: Average is 190 mL/g (2)

K_d: 1.36 mL/g for a sandy loam with 1.1% OM and pH 7.3; 2.53 mL/g for a silty clay loam with 2% OM and pH 5.3; 0.64 mL/g for a sandy clay loam with 1.5% OM and pH 6.4

Transformation:

Photodegradation: Minimal losses

Other degradation: Cyanazine is primarily degraded by soil microbes converting the nitrile to an amide group with further oxidation to the carboxylic acid. Non-microbial hydrolysis producing hydroxy cyanazine occurs rapidly at low soil pH but slowly at high pH.

Persistence: Cyanazine has somewhat short soil residual activity with an average field half-life of 14 d (2).

Field/lab experiments: In sandy loam soils with ~1% OM, half-life is 12-15 d, depending on temperature and soil moisture. In silt loam and clay loam soils with 2.8-3.0% OM, half-life is 20-25 d. Half-life is shorter at pH <5.5 and longer at pH>7.5

Mobility: Leached 11.4 cm with 5 cm of applied water in a sandy loam soil

Volatilization: Minimal losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cyanazine unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 182-334 mg/kg; mouse, 380 mg/kg; rabbit, 141 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; rat, >1200; 4-h inhalation LC_{50} rat, >0.809 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, none

BLADEX 90 DF: Oral LD_{50} male rat, 313 mg/kg; female rat, 238 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 1-h inhalation LC_{50} rat, 0.809 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe

BLADEX 4L: Oral LD_{50} rat 475-510 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 1-h inhalation LC_{50} rat, 0.089-0.548 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, rat: NOEL 10 mg/kg/d; weight effects

Chronic toxicity:

24-mo dietary, rat: NOEL 12 mg/kg/d; mammary adenoma/carcinoma

24-mo dietary, dog: NOEL 25 mg/kg/d; body weight and blood chemistry effects

Teratogenicity:

Rat and rabbit: NOEL NA; developmental effects at maternally toxic doses in 1 of 2 strains

Reproduction:

Rat: NOEL 25 mg/kg/d; body weight effects

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: *In vitro* cytogenetics, negative; Mouse lymphoma, positive

DNA damage/repair: *In vivo* mouse/UDS, negative; *In vitro* UDS, positive.

Wildlife:

Bobwhite quail oral LD_{50}, 400 mg/kg; Mallard duck oral LD_{50}, >2000 mg/kg; Honey bee, not toxic; Daphnia 48-h LC_{50}, 49 mg/L; Bluegill sunfish 96-h LC_{50}, 23 mg/L; Rainbow trout 96-h LC_{50}, 9 mg/L; Harlequin fish 96-h LC_{50}, 7.5 mg/L; Sheepshead minnow 48-h LC_{50}, 18 mg/L

Use classification: Restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React cyanuric chloride and aminoisobutyronitrile.

Purification of technical: Crystallization from acetone

Analytical methods: By IR spectroscopy, GLC, or HPLC

Historical: Discovered by Werner Schworze in Germany. First reported in 1967 (1). Patented as a herbicide in November 1971. Introduced by Shell Research Ltd; Great Britain patent 1,132,306. Developed in the U.S. by Shell Development Company and sold from 1971-86. Marketed from 1987-present in the U.S. by Du Pont Company.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

1. Hughes, W. J. et al. 1967. Proc. North Cent. Weed Control Conf. p. 27.
   Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

cycloate

CAS #: 1134-23-2 **N**$^{(8)}$

S-ethyl cyclohexylethylcarbamothioate

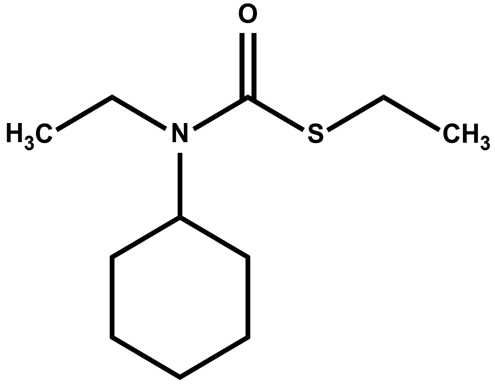
NOMENCLATURE

Common name: cycloate (BSI, ISO, WSSA)
Other name(s): R-2063; hexylthiocarbam; S-ethyl cyclohexyl(ethyl)thiocarbamate (IUPAC); S-ethyl N-ethylthiocyclohexanecarbamate
Trade name(s): MARATHON; RO-NEET ®
Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

Cycloate



Molecular formula: $C_{11}H_{21}NOS$
Molecular weight: 215.35 g/mole
Description: Liquid at room temperature, aromatic odor
Density: 1.02 g/mL (20 C)
Melting point: NA
Boiling point: 145-146 C (1.33×10^{3} Pa)
Vapor pressure: 8.2×10^{-1} Pa (25 C)
Stability: Stable for 6 wk (54.5 C)
Solubility:
water 85 mg/L (22 C)
organic solvents g/100 mL (20 C):
acetone >100
xylene >100
benzene miscible
kerosene miscible
ethanol >100
methylisobutyl ketone >100
4-methylpentan-2-one miscible
pK$_a$: None (non-ionizable)
K$_{ow}$: 13,000 (25 C)

HERBICIDAL USE

Cycloate can be applied spring PPI at 2.8-4.5 kg ai/ha in sugarbeets, fall PPI at 3.4-4.5 kg ai/ha in sugarbeets planted the following spring, and PPI at 3.4-4.5 kg ai/ha in table beets and spinach. It primarily controls annual grasses such as barnyardgrass, crabgrass spp., foxtail spp., and wild oats, but also controls certain annual broadleaf weeds including lambsquarters, purslane, and redroot pigweed. Cycloate can be applied by conventional sprayer, impregnated on dry bulk fertilizer, or banded by soil injection equipment.

USE PRECAUTIONS

Fire hazard: RO-NEET 6-E is non-flammable, but has moderate fire hazard; flash point is 139 C (TOC); fire point is 149 C.
Corrosiveness: RO-NEET 6-E is non-corrosive
Storage stability: RO-NEET 6-E is stable for 16 h at 100 C and 3.6 yr at room temperature; freezes at -6.7 C
Cleaning glassware/spray equipment: Wash glassware with acetone followed by water; flush equipment with water.
Emergency exposure: If ingested, do not induce vomiting. Wash skin with soap and water. Rinse eyes with running water for 15 min.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Suspected to be inhibitors of fatty acid and lipid biosynthesis (more details on page 13)
Symptomology: Susceptible weeds typically fail to emerge as the grass coleoptile or broadleaf hypocotyl ceases growth beneath the soil. Injury on tolerant grass species may appear as twisted and malformed stems with leaves tightly rolled in the whorl and unable to unroll normally. Leaves do not emerge properly from the coleoptile and may do so underground. Broadleaf seedlings may have slightly cupped or crinkled leaves and shortened leaf midribs producing a “drawstring” effect on the leaf tip.
Absorption/translocation: Soil-applied cycloate is readily absorbed by sugarbeet roots and translocated upward to the stems and leaves. Foliar-applied cycloate also is rapidly absorbed by leaves, although it is not POST-applied in the field.
Metabolism in plants: Sugarbeet roots and leaves rapidly metabolize cycloate to ethyl-cyclohexylamine, CO_2, amino acids, sugars, and other compounds. Sugarbeets metabolized all cycloate residues by 3 d after application.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed
K$_{oc}$ and K$_d$: K$_{oc}$ 600 mL/g and K$_d$ 9 mL/g for adsorption, and K$_{oc}$ 767 mL/g and K$_d$ 11.5 mL/g for desorption in a silt loam with 1.5% OM; K$_{oc}$ 500 mL/g and K$_d$ 10 mL/g for adsorption, and K$_{oc}$ 615 mL/g and K$_d$ 12.3 mL/g for desorption in a loam with 2% OM; K$_{oc}$ 545 mL/g and K$_d$ 2.18 mL/g for adsorption, and K$_{oc}$ 745 mL/g and K$_d$ 2.98 mL/g for desorption in a sandy loam with 0.4% OM; K$_{oc}$ 678 mL/g and K$_d$ 8.13 mL/g for adsorption, and K$_{oc}$ 803 mL/g and K$_d$ 9.63 mL/g for desorption in a clay with 1.2% OM
Transformation:
Photodegradation: Half-life is 219 d in water. Photolysis is a relatively unimportant contributor to field dissipation

of cycloate.

Other degradation: Microbial breakdown is responsible for a large part of the disappearance of cycloate from soils when incorporated in the soil to a depth of 5-7.6 cm.

Persistence: Average field half-life is 30 d (4). Half-lives of 4-8 wk have been measured across several soils under field conditions.

Lab experiments: Half-life was 3.5 wk in a loam soil at 21-27 C

Mobility: Cycloate resists leaching in soils high in clay or OM, but has moderate to high leaching potential in soils low in clay and OM. It leached 7.6-15.2 cm with 20 cm of water applied to loamy sand. Cycloate leaches slightly less than EPTC and pebulate.

Volatilization: Substantial losses when left on the surface of moist soils, but little is lost when left on a dry soil surface.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cycloate unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 3200 mg/kg; female rat, 2275 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 0.0047 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, weak;

Eye irritation rabbit, mild

RO-NEET 6-E: Oral LD_{50} male rat, 3160 mg/kg; female rat, 3690 mg/kg; Dermal LD_{50} rabbit, >4640 mg/kg; 4-h inhalation LC_{50}, 5.03 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, rat: NOEL 55 mg/kg/d

90-d dietary, dog: NOEL 240 mg/kg/d

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Japanese quail LD_{50}, >2000 mg/kg; Honey bee non-toxic; Rainbow trout 96-h LC_{50}, 4.5 mg/L

RO-NEET 6-E: Bobwhite quail 7-d dietary LC_{50}, >56,000 ppm; Mosquito fish 96-h LC_{50}, 10 mg/L; Rainbow trout 96-h LC_{50}, 5.6 mg/L

Use classification: General use for all products

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Ethyl chlorothioformate is reacted with ethyl cyclohexyl amine and base

Purification of technical: NA

Analytical methods: Cycloate can be separated from impurities on several columns and determined by GC with thermal conductivity, flame ionization or mass spectrometry.

Historical: Introduced by Stauffer Chemical Company; U.S. patent 3,175,897.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Casida, J. E. et al. 1974. Science 184:573.
2. Fuerst, E. P. 1987. Weed Technol. 1:270.
3. Gronwald, J. W. 1991. Weed Sci. 39:435.
4. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

cyclosulfamuron

CAS #: 136849-15-5 $2^{(B)}$

N-[[[2-(cyclopropylcarbonyl)phenyl]amino] sulfonyl]-N'-(4,6-dimethoxy-2-pyrimidinyl)urea

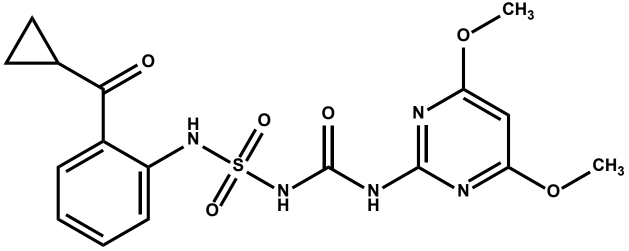
NOMENCLATURE

Common name: cyclosulfamuron (ANSI, ISO, WSSA)
Other name(s): AC 322,140; CL 322,140 (code numbers); 1 {[*o*-(cyclopropylcarbonyl)phenyl]sulfa-moyl}-3-(4,6-dimethocy-2-pyrimidinyl)-urea (IUPAC)
Trade name(s): ICHIYONMARU® JUMBO GR: NEBIROSU
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

cyclosulfamuron



Molecular formula: $C_{17}H_{19}N_5O_6S$
Molecular weight: 421.43 g/mole
Description: Odorless, off-white solid
Density: 0.794 g/mL (tapped); 0.66 g/mL (22.4 C)
Melting point: 169-175 C (technical)
Boiling point: NA
Vapor pressure: <2.2 x 10^{-5} Pa (20 C)
Stability: Technical grade material was not observed to be sensitive to oxidizing or reducing agents, but it hydrolyzes rapidly.
Solubility:
water (25 C), 0.14 mg/L (pH 5); 5.79 mg/L (pH 7); 579 mg/L (pH 9)
organic solvents g/100mL (20 C):
n-hexane 0.0001
toluene 0.11
dichloromethane 4.3
acetone 2.1
pK$_a$: 5.04 (weak acid)
K$_{ow}$: 733 (pH 5.0); 70.4 (pH 6.0); 37.6 (pH 7.0); 3.96 (pH 8.0); 1.05 (pH 9.0)

HERBICIDAL USE

Cyclosulfamuron at 45-60 g ai/ha controls a wide range of broadleaf weeds and sedges. It exhibits good selectivity on cereals and rice and is active when applied PRE or POST.

USE PRECAUTIONS

Fire hazard: Cyclosulfamuron is not flammable (10% WP)
Corrosiveness: Slightly corrosive of aluminum
Storage stability: > 18 mo (25 C)
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent.
Emergency exposure: In case of skin contact, wash affected area with copious amounts of soap and water. In case of eye contact flush with water for at least 15 mins. In case of ingestion, consult a physician.
Incompatibilities: Unstable with high alkaline pesticides

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more detalis on page 12)
Symptomology: Following POST applications, susceptible weeds cease growing, becoming chlorotic and die. Depending upon environmental conditions, complete death of treated plants may take several weeks.
Absorption/translocation: Cyclosulfamuron is readily absorbed by plant roots and foliage and is translocated throughout the plant.
Metabolism in plants: Crops such as rice, wheat, barley, and turf metabolize this herbicide rapidly (half-life <4 hours) and are very tolerant to cyclosulfamuron. Susceptible plants do not metabolize the herbicide as rapidly.

BEHAVIOR IN SOIL

Sorption: Cyclosulfamuron is strongly to moderately adsorbed to soil particles.
K$_d$: 4.6 mL/g
Transformation:
Photodegradation: Cyclosulfamuron is rapidly degraded in water under photolytic conditions
Other degradation: Cyclosulfamuron is degraded by microbial and hydrolytic pathways. The rate of degradation is influenced by soil pH and degradation occurs more rapidly at low soil pH.
Persistence: Soil half-life is about 2 mo at pH 6.1 under aerobic conditions. Longer half-lives occur at higher soil pH.
Mobility: Soil bioassays have shown that cyclosulfamuron is non-mobile and remains in the upper 1 to 3 cm of soil columns.
Volatilization: Low or negligible
Formulation effects: Granular formulation carriers are used in paddy rice.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cyclosulfamuron unless otherwise indicated.
Acute toxicity:
Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rat, >4000 mg/kg; Primary eye irritation rabbit, slightly irritating; Skin irritation rabbit, negative
Subchronic toxicity:
90-d dietary, mouse: NA
90-d dietary, rat: 1000 mg/kg or 81 mg/kg/d

90-d dietary, dog: 1000 mg/kg or 30 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL >7000 mg/kg or >1236 mg/kg/d (male); >566 mg/kg/d (female)

24-mo dietary, rat: NOEL 1000 mg/kg or 50 mg/kg/d (male); 63 mg/kg/d (female)

12-mo dietary, dog: NOEL 100 mg/kg or 3 mg/kg/d

Teratogenicity:

Rat : >1000 mg/kg/d (oral)

Rabbit: NOEL 100 mg/kg/d (maternal); NOEL >1000 mg/kg/d (fetal)

Reproduction:

Rat: NOEL >20000 mg/kg or >1550 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, nonmutagenic; CHO, negative

Structural chromosome aberration: Negative

DNA damage/repair: Negative

Other unidentified tests: Negative

Wildlife:

Daphnia 48-h EC_{50}, >9.1 mg/L; Rainbow trout 96-h LC_{50}, >7.7 mg/L; Carp 96-h LC_{50}, >7.0 mg/L

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Cyclosulfamuron was developed by American Cyanamid Agricultural Research Division, Princeton, NJ. The herbicide was registered for use in Japan in 1997.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF

cycloxydim

CAS #: 01205-02-1

1 **(A)**

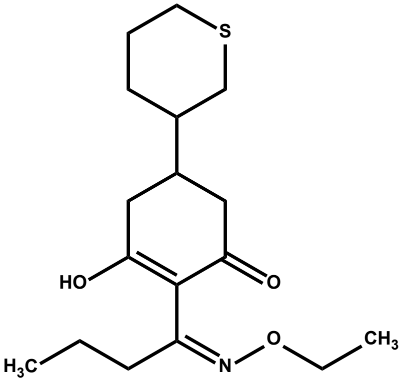
2-[1-(ethoxyimino)butyl]-3-hydroxy-5-(tetrahydro-2H-thiopyran-3-yl)-2-cyclohexen-1-one

NOMENCLATURE

Common name: cycloxydim (ISO)
Other name(s): BAS 517H; (5RS)-2-[(EZ)-1-(ethoxyimino)butyl]-3-hydroxy-5-[(3RS)-thian-3-yl]cyclohex-2-en-1-one
Trade name(s): FOCUS; LASER; STRATOS
Chemical family: cyclohexanedione; cyclohexane-dione oxime; cyclohexenone; cyclohexene oxime

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *cycloxydim*



Molecular formula: $C_{17}H_{27}NO_3S$
Molecular weight: 325.47 g/mole
Description: Amber-colored oily liquid, weakly aromatic
Density: 1.165 g/mL (20 C)
Melting point: 37 C (technical grade)
Boiling point: NA
Vapor pressure: 1.33×10^{-5} Pa (20 C)
Stability: Decomposes at 127 C; degraded by UV light
Solubility:
- water 53 mg/L (pH 4.3, 20 C)
- organic solvents g/100 mL (20 C)
- acetone >126
- n-hexane >151
- benzene 114
- methanol >126
- ethyl acetate >111
- dichloromethane >25
- toluene >25

pK_a: 4.17 (weak acid)
K_{ow}: log K_{ow} = 1.36 (pH 7, 25 C)

HERBICIDE USE

Cycloxydim can be applied POST at 0.056-0.448 kg ai/ha for control of annual and perennial grasses with essentially no control of broadleaf species. An oil adjuvant or surfactant is recommended for maximum efficacy. Cycloxydim is not registered in the U.S. but is used in certain other countries.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable for at least 1 yr
Cleaning glassware/spray equipment: Wash with detergent
Emergency exposure: Wash skin with soap and water. Poisoning symptoms include apathy, staggering, paresis, tremors, or twitching.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase). (morel details on page 12)
Symptomology: Growth ceases within a few d of application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop within 1-3 wk of application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.
Absorption/translocation: Readily absorbed into foliage when applied with an oil adjuvant. Rainfall 1 h after application does not reduce efficacy. Foliar-absorbed BAS 517 H translocates in the phloem and accumulates in meristematic regions. Acropetal translocation of root-absorbed BAS 517 H also occurs.
Metabolism of plants: Soybeans rapidly oxidize and conjugate cycloxydim
Non-herbicial biological properties: Stimulates increased sugar content of sugarcane at harvest
Mechanism of resistance in weeds: Most weed biotypes that have developed resistance to aryloxyphenoxy propionates with cross-resistance to the cyclohexanediones appear to have an ACCase that is insensitive to the herbicide.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed on all soils
Transformation: NA
Photodegradation: NA
Other degradation: NA
Persistence: Very short soil residual life, but half-life varies with environmental conditions. Grasses may be controlled when emerging immediately after application.
Lab experiments: Half-life at room temperature was 0.58 d in a loamy sand (pH 6.0) and 0.5 d in a sandy loam (pH 6.6)
Mobility: Low leaching rates
Volatilization: Minimal losses.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cycloxydim unless otherwise indicated.

Acute toxicity:

Oral LD_{50} mouse, >5000 mg/kg; Oral LD_{50} rat, >3940 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50}, for rats >5.28 mg/l; Skin irritation rabbit, none; Skin sensitization, guinea pig, no; Eye irritation rabbit, none

Subchronic toxicity:

90-d dietary, rat: NOEL 25 mg/kg/; decreased gain and food consumption; alternations in clinical-chemical parameters

90-d dietary, dog: NOEL 50 mg/kg; target organ: liver and red blood cells, alternations in clinical-chemical parameters

Chronic toxicity:

Dog: NOEL 12 mg/kg; target organ: liver including histopathological changes and red blood cells

Rat: NOEL 7 mg/kg; reduced gain and altered clinical-chemical parameters

Carcinogenicity: Non-carcinogenic in rat. Not carcinogenic in mouse (NOEL 32 mg/kg)

Teratogenicity:

Rat: Maternal and developmental NOEL: 200 mg/kg; not teratogenic

Rabbit: Maternal NOEL: 100 mg/kg, developmental NOEL 400 mg/kg; not teratogenic

Reproduction:

Rat: NOEL (parental toxicity) 9.7 mg/kg; NOEL (developmental toxicity) 37.8 mg/kg; NOEL (reproduction) >129 mg/kg

Mutagenicity:

Gene mutation: Ames test and CHO/HPRT test: negative

Structural chromosome aberrations: In vitro (CHO cells), and in vivo (Chinese Hamster bone marrow and Micro Nucleus Test, mouse): overall conclusion: not mutagenic

DNA damage and repair: In vitro UDS assay: negative

Wildlife: Low toxicity to birds, fish, pollinating insects, and aquatic invertebrates

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Confidential

Purification of technical: Contact BASF

Analytical methods: Contact BASF

Historical: Cycloxydim was discovered and developed by BASF. It was first tested in the US in 1984.

MANUFACTURER(S) AND INFORMATION SOURCES

Industry source(s): BASF

Reference(s):

1. Burton, J. D. et al. 1989. Pestic. Biochem. Physicol. 34:76.
2. Focke and Lichtenthaler. 1987. Z. Naturforsch. 42c:1361.

cyhalofop-butyl

(2R)2-[4-(4-cyano-2-fluorophenoxy)phenoxy]propanoate butyl ester

CAS # Acid: 122008-8-0
Butyl ester: 122008-85-9

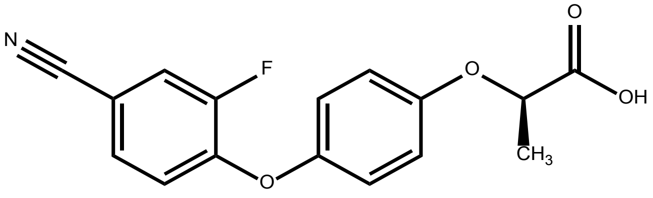
1$^{(A)}$

NOMENCLATURE

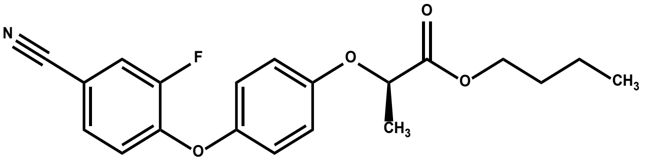
Common name: cyhalofop-butyl; (ISO approved)
Other name(s): DE-537; XDE-537; XRD-537; DEH-112; (Acid) (R)-2-[4-(4-cyano-2-fluorophenoxy) phenoxy] propionic acid (IUPAC); cyhalofop-butyl (butyl ester); (Butyl ester) butyl(2R)-2-[4-(4-cyano-2-fluorophenoxy)phenoxy] propanoate (IUPAC)
Trade name(s): BARNSTORM; CLINCHER® CA; CLINCHER® SF; CLINCHER® EZ; CLINCHER® EC; CLINCHER® GRANULE; REBELEX™; CRANSTAN EC
Chemical family: aryloxyphenoxy propionate; aryloxyphenoxy propionic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:



Cyhalofop acid



Cyhalofop butyl ester

Molecular Formula: Acid $C_{16}H_{12}FNO_4$; Butyl ester $C_{20}H_{20}FNO_4$
Molecular weight: Acid 301.27 g/mole; Butyl ester 357.4 g/mole
Description: White crystalline solid
Density: 1.17 g/mL (20 C)
Melting point: 45.5 to 49.5 C
Vapor pressure: 5.3 x 10^{-5} Pa (25 C); Henry's Law constant 9.51 x 10^{-4} Pa m^3 mol^{-1}
Stability: No chemical degradation was observed at elevated temperatures
Compatibility: No chemical degradation was observed in the presence of metals and metal ions
Solubility: Unbuffered water, 0.44 mg/L (20 C); 0.46 mg/L (pH 5, 20 C); 0.44 to 0.7 mg/L (pH 7, 20 C); acetonitrile, >250 g/L; n-Heptane, 6.06 g/L; n-octanol, 16.0 g/L; dichloroethane, >250 g/L; methanol, >250 g/L; acetone, >250 g/L; ethyl acetate, >250 g/L
K_{ow}: log K_{ow} = 3.32 (25 C)

HERBICIDAL USE

Cyhalofop-butyl is a postemergence herbicide for selective control of grass weeds in dry-seeded and water-seeded rice. Common postemergence use rates are 210 to 310 g ai/ha.

Cyhalofop-butyl controls a wide spectrum of annual and seedling perennial grasses in rice with excellent rice safety and low drift hazard to neighboring row crops.

Cyhalofop-butyl has no preemergence or soil residual activity, and only grass weeds emerged at the time of application are controlled. Cyhalofop-butyl will not control broadleaf weeds or sedges. When used as a postemergence foliar application, cyhalofop-butyl is mixed with a crop oil concentrate or surfactant for maximum effectiveness. In flooded paddy trans-planted rice markets (California water-seeded, and Japan/Korea transplanted rice), cyhalofop-butyl is formulated as a granule, either alone or in combination with other products. Granules are applied directly to flooded rice paddies for selective control of weeds.

USE PRECAUTIONS

Fire hazard: Flashpoint of U.S. EC formulation: 45 C
Storage stability: Material is stable under recommended storage conditions. Product can decompose at elevated temperatures.
Emergency exposure: Wash skin with flowing water or shower. Irrigate eyes with water for at least 15 minutes and seek medical attention. If swallowed, seek medical attention. Do not induce vomiting unless directed to do so by medical personnel.
Irritant: May cause moderate eye irritation; may cause corneal injury
Incompatibilities: Avoid contact with oxidizing materials

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase). (more details on page 12)
Symptomology: Grass weeds cease growth immediately after treatment. Yellow patches appear within 2-3 days to one week, first on the youngest leaves, and then on older leaves later, leading to necrosis and death of the whole plant within two to three weeks depending on size of weeds when treated and weather conditions. Senescent pigment changes (reddening) are often observed in older leaves due to a loss of membrane integrity. Root growth is also inhibited. The time required for complete kill is shortest under high temperature/high moisture conditions.
Absorption/translocation: Cyhalofop-butyl is readily absorbed by plant tissue, is moderately phloem mobile, and accumulates in the meristematic region of the plant. In early to beginning tillered grass weeds, it does not translocate readily. Rapid absorption with translocation to the meristem ensures reliable control of non-tillered grasses with cyhalofop-butyl. Commercial liquid formulations are rainfast within 2 to 3 h after treatment. The foliar systemic activity of cyhalofop-butyl together with inhibition of meristematic activity assures control of a wide range of grass weed sizes from 1 leaf through tillering, depending on rate of application,

weed species, and weed size.

Metabolism in Plants: Rice tolerance to cyhalofop-butyl is due to a rapid metabolism to the herbicidally inactive diacid ($t_{1/2}$ < 10 hr) and to subsequent formation of polar and non-polar metabolites. Conversely, in susceptible grasses such as barnyardgrass (Echinochloa crus-galli), herbicidal efficacy is attributed to the biologically active monoacid form (80% conversion within < 10 hr).

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 2066 - 9637 mL/g indicate that cyhalofop-butyl is strongly adsorbed to soil

Mobility: Very low due to strong adsorption

Transformation:

Photodegradation: Insignificant.

Other degradation: Cyhalofop-butyl was more stable at pH 5 but hydrolyzed quickly at pH 9 ($t_{1/2}$ = 0.4 d)

Persistence: Soil microorganisms actively degrade cyhalofop-butyl. Laboratory metabolism studies have shown that the half-life of cyhalofop-butyl is <1 day (typically 0.1-0.2 day) under aerobic and anaerobic conditions in both soil and aquatic systems. The metabolites of cyhalofop-butyl are cyhalofop-acid, cyhalofop-amide and cyhalofop-diacid, and are also transient in the environment, with half-life values of <4 days in aerobic soil systems and 7-40 days in aerobic aquatic systems, and are almost completely degraded within 30 days, terminating in evolution of CO_2 and incorporation into natural organic matter. A two-site aquatic field dissipation study using both dry-seeded and paddy seeded rice growing conditions confirmed the rapid degradation of cyhalofop-butyl. The combination of rapid dissipation and strong sorption to soil (Kd values range from 17.8 to 138 mL/g) indicates that cyhalofop-butyl will not be mobile within soil and will not pose a risk to groundwater. The rapid environmental dissipation of cyhalofop-butyl and its metabolites results in minimal environmental exposure to non-target organisms and minimal potential for transport away from the site of application.

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade cyhalofop-butyl unless otherwise indicated. Acute toxicity testing of cyhalofop-butyl technical places this active ingredient almost exclusively in toxicity class IV. Subchronic, chronic, and reproductive, developmental toxicity testing revealed no significant adverse effects. A series of mutagenicity tests were negative, no adverse findings determined in neurotoxicity studies, and no adverse effects shown in oncogenicity studies

Acute toxicity (LD_{50}):

Oral, rat (male/female), >5,000 mg/kg; Dermal, rats, >5,000 mg/kg; Eye irritation rabbit, slight irritation (reversible); Skin irritation rabbit, No irritation; Skin sensitization, guinea pig, negative; Inhalation LC_{50},rat, >5.63 mg/L

Mutagenicity:

Ames-test: Negative

Chromosomal aberration: Negative

Micronucleus test: Negative

Wildlife:

Clincher CA: Bobwhite quail LD_{50}, >2250 mg/kg; Mallard duck LD_{50}, >2250 mg/kg; 8-d dietary, Mallard duck LC_{50}, >5620 mg/kg; Bobwhite quail LC_{50}, >5620 mg/kg; Bluegill sunfish (96-h) LC_{50}, 0.789 mg/L; Rainbow trout (96-h) LC_{50}, 1.48 mg/L; Daphnia magna (48-h) LC_{50}, >2.7 mg/L; oyster EC_{50}, 0.52 mg/L; honeybee LD_{50}, > 100 ug/bee; compound has low toxicity to terrestrial organisms including birds, non-target insects and earthworms. Toxicity to fish, aquatic invertebrates and algae is at, or above, the water solubility of cyhalofop-butyl.

History:

Cyhalofop-butyl was discovered in the mid 1980's by the Dow Chemical Company and was first introduced into the marketplace in 1996. As of 2013, Dow AgroSciences holds global registrations in many key rice-growing regions including Japan, other Asian countries, the European Union, Middle East, Africa and Latin America. Registration was granted in the United States in 2002 and USEPA Registration Review is anticipated to begin in 2014

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purifications of technical: NA

Analytical methods: Residues of cyhalofop-butyl and its metabolites, cyhalofop acid and cyhalofop diacid, are extracted from agricultural commodities by homogenizing and shaking with acetone/1N HCl (80/20, v/v). An aliquot of extract is then hydrolyzed with 3.5 mL 1N NaOH, and then was subjected to reversed-phase solid-phase extraction (SPE) purification. The SPE eluate is evaporated to dryness, and reconstituted in 2.0 mL acetonitrile/water (25/75, v/v) containing 0.01% formic acid. The cyhalofop-butyl is hydrolyzed into cyhalofop acid during the process, and is quantified as cyhalofop acid equivalent. The final sample is analyzed for cyhalofop acid and cyhalofop diacid by liquid chromatography coupled with negative-ion electrospray tandem mass spectrometry (LC-MS/MS).

MANUFACTURER(S) AND INFORMATION SOURCES

Industry source(s): Dow AgroSciences

cyprosulfamide

CAS #: 221667-31-8: **NC**

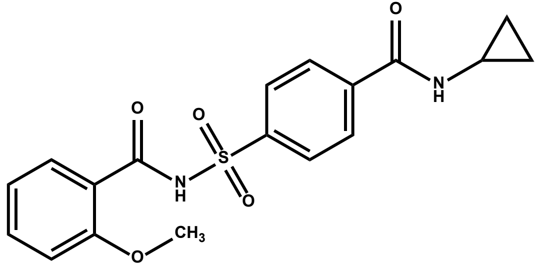
N-[[4-[(cyclopropylamino)carbonyl]phenyl]sulfonyl]-2-methoxybenzamide

NOMENCLATURE

Common name: Cyprosulfamide
Other name(s): *N*-[4-(cyclopropylcarbamoyl) phenylsulfonyl]-o-anisamide (IUPAC)
Trade name(s): BALANCE FLEXX, CORVUS
Chemical family: NA

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
cyprosulfamide



Molecular formula: $C_{18}H_{18}N_2O_5S$
Molecular weight: 374.41 g/mole
Description: white powder
Density: 1.51 g/cm^3 at 20 C
Melting point: 218 *C*
Boiling point: NA
Vapor pressure: Pa (25 C) NA
Stability: NA
Solubility:NA
Water:
0.0034 g/l
Organic solvents
Acetone 3.1 g/l at 20 C
pH: 3.9 at 0.1 g/l at 23 C
K_{ow}: log K_{ow} = -0.8 at 23 C

HERBICIDAL USE

Cyprosulfamide is used as a safener for isoxaflutole in corn.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable under recommended storage conditions
Cleaning glassware/spray equipment: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Cyprosulfamide accelerates herbicide detoxification in certain plants.
Symptomology: NA
Absorption/translocation: NA
Metabolism in plants: NA
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Photodegradation: NA
Other degradation: NA.
Persistence: NA
Field experiments: NA
Mobility: NA
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Acute toxicity: Rat: oral LD_{50} >2,000 mg/kg
LC_{50} Inhalation-rat: >3.5 mg/l
LD_{50} Dermal-rat >2000 mg/kg
No skin irritaiton (rat),
No eye Irritation (rabbit)
Does not cause skin sensitisation (guinea pig)
Subchronic toxicity: NA
Chronic toxicity: rat-repeated dose toxicity NOEL 58 mg/kg; LOEL 240 mg/kg; mouse 90 d feeding study NOEL >1110 mg/kg; dog 365 d feeding study NOEL 66 mg/kg LOEL 226 mg/kg.
Teratogenicity: Non-teratogenic
Reproduction: NA
Mutagenicity: Non-mutagenic
Wildlife:
minnow LC_{50} >102 mg/l; Water flea LC_{50} 102 mg/l (48 h); *Lemna minor* EC_{50} >104 mg/L (7 d); green algae EC_{50}> 99.7 mg/l (96 h)
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer Crop Science

dazomet

CAS #: 533-74-4 **$26^{(Z)}$**

tetrahydro-3,5-dimethyl-2*H*-1,3,5-thiadiazine-2-thione

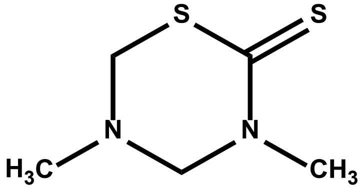
NOMENCLATURE

Common name: dazomet (BSI, ISO, WSSA)
Other name(s): N-521; tiazon; tetrahydro-3,5-dimethyl-1,3,5-thiadiazine-2-thione or 3,5-dimethyl-1,3,5-thiadiazinane-2-thione (IUPAC)
Trade name(s): BASAMID® G; MYLONE
Chemical family: dithiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

dazomet



Molecular formula: $C_5H_{10}N_2S_2$
Molecular weight: 162.27 g/mole
Description: White crystalline solid, odorless
Density: NA
Melting point: 100-106 C
Boiling point: NA
Vapor pressure: 3.7×10^{-4} Pa (20 C)
Stability: Decomposes above 102 C
Solubility:

water 2000 mg/L (20 C)
organic solvents g/100 mL:
acetone 13.1
benzene 4.5
chloroform 30
dioxane 8
dimethylformamide 30
DMSO 30
ethanol 3
ethylene glycol 3
isopropanol 0.5
methanol 3
trichloroethylene 30
p-xylene 1.1
ethylene glycol monethylether 5

pK_a: None (non-ionizable)
K_{ow}: 1.4 (pH 7)

HERBICIDAL USE

Dazomet can be applied PPI as a soil fumigant at 194-588 kg ai/ha in tobacco seedbeds, ornamental seedbeds and fields, forest tree seedbeds, potting soil, turf seedbeds, and for turf renovation. Soil must be kept moist for 5-7 d after application. Dazomet controls soil-borne pathogens, germinating weed propagules, and nematodes.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: NA
Storage stability: Stable at ambient temperatures if kept dry; gradual endothermic decomposition above 102 C
Cleaning glassware/spray equipment: Clean equipment with water
Emergency exposure: If ingested, induce vomiting with large amounts of water; get medical attention; for small doses, give activated charcoal and follow in 3-4 h with sodium sulfate as a cathartic; for large doses, lavage stomach. Dust may irritate skin and eyes.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Dazomet may interact with nucleophilic centers, e.g. thiol groups, in enzymes and proteins (1). Also, dazomet inhibits activity of the Cu^{2+}-containing enzyme *o*-diphenoloxidase in potato and other organisms (3). These findings suggest that dazomet may complex Cu necessary for *o*-diphenoloxidase activity and could complex other metals important to the activity of several enzymes.. (more details on page 15)
Symptomology: Dazomet delays emergence or kills seedlings before emergence from the soil. Dormant seeds or seeds with impermeable seed coats may not be killed by dazomet.
Absorption/translocation: Absorbed through the seed coat or into root and shoot tissues of emerging weed seedings
Metabolism in plants: Dazomet decomposes in soil to methyl isothiocyanate, formaldehyde, hydrogen sulfide, and monomethylamine. Methyl isothiocyanate probably is the most phytotoxic and is absorbed by emerging seedlings.
Non-herbicidal biological properties: Dazomet has soil sterilant properties in controlling fungi, nematodes, and soil insects, as well as weeds. It also is used in slimicides and in adhesives and glues for production of paper, paperboard, and other paper products.
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:
K_{oc}: Average is 10 mL/g (estimated) (1)
Transformation:
Photodegradation: Negligible losses
Other degradation: Dazomet is made active in soil by decomposition to methyl isothiocyanate, formaldehyde, hydrogen sulfide, and monomethylamine. The most active of these degradation products appears to be methyl isothiocyanate. Biological activation of dazomet requires soil moisture and its decomposition rate depends on soil characteristics, humidity, and temperature. Under normal soil conditions, the degradative activation of dazomet occurs within 10-15 min after application.
Persistence: Average field half-life is 7 d (1). Dazomet does not accumulate in the soil.
Mobility: NA
Volatilization: Significant losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dazomet unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 650 mg/kg, male mouse, 455 mg/kg, female mouse, 710 mg/kg; Dermal LD_{50} rabbit, 320-620 mg/kg; 4-h inhalation LC_{50} rat, 8.4 mg/L

Subchronic toxicity:

90-day dietary, rat: NOEL 1.5 mg/kg/d (males), 5.4 mg/kg/d (females); decreased body weight gain, increased liver weight, fatty degeneration in liver

21-day dermal, rabbit: NOEL > 1000 mg/kg/d; no systemic effects

Chronic toxicity:

18-month dietary, mouse: NOEL 5 mg/kg/d; slight increase in hepatocellular adenomas (females). Not carcinogenic

24-month dietary, rat: NOEL 1.0 mg/kg/d; decreased body weight, decreased serum cholinesterase, anemia, increased liver weight, hepatocellualr fatty deposition and vacuolation (females)

12-month dietary, dog: NOEL 1.6 mg/kg/d (males) 0.5 mg/kg/d (females); chronic hepatitis, cirrhosis

Teratogenicity:

Rat: NOEL maternal and developmental 3.0 mg/kg/d; maternal reduced body weight gain and reduced pup weight; not teratogenic

Rabbit: NOEL maternal >25 mg/kg/d, developmental 12.5 mg/kg/d; No maternal toxicity; embryolethality at highest dose; not teratogenic

Reproduction:

Rat: NOEL parental 1.0 mg/kg/d, reproductive and developmental > 18 mg/kg/d; parental reduced body weight and liver toxicity; no reproductive or developmental effects

Mutagenicity:

Gene Mutation: Ames test negative; CHO/HGPRT positive

Structural chromosome aberration: Human lymphocyte *in vitro* negative; mouse micronucleus negative; mouse lymphoma negative with S-9, positive without S-9; *in vivo* cytogentetics negative; spermatogonia negative

DNA damage/repair: *B. subtilis* REC assay negative; rat *in vivo/in vitro* UDS assay negative; rat hepatocyte UDS equivocal

Wildlife:

Bobwhite quail oral LD_{50}, 415 mg/kg; Honey bee, nontoxic; Rainbow trout 96-h LC_{50}, 0.16 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React carbon disulfide, methylamine, and caustic soda. See Chem. Week 79(18):82-83 (1956).

Purification of technical: NA **Analytical methods:** Dazomet is hydrolyzed in dilute acid medium to carbon disulfide, formaldehyde, and methylamine. Evolved carbon disulfide is absorbed in ethanolic cupric acetate, diethylamine, and triethanolamine. Color intensity of the resulting diethyldithiocarbamate is measured photometrically at 385 nm.

Historical: Originally prepared in 1897 and later introduced as a soil fumigant (2). Introduced in 1952 by BASF.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Certis USA, L.L.C.; Hopkins Agricultural Chemical Co.

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Cremlyn, R. J. 1991. Agrochemicals: Preparation and Mode of Action. Wiley and Sons, New York.
3. Delepine, M. 1897. Bull. Soc. Chim. Fr. 15:891.
4. Vaughan and Ord. 1979. New Phytol. 83:361.

DCPA

CAS #: 1861-32-1 $3^{(K_1)}$

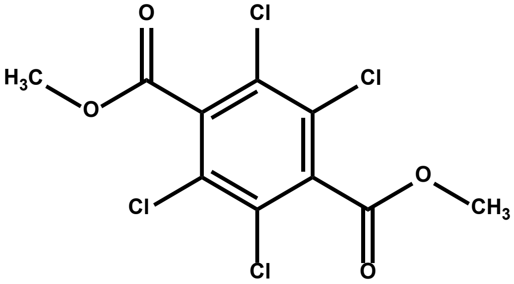
dimethyl 2,3,5,6-tetrachloro-1,4-benzenedicarboxylate

NOMENCLATURE

Common name: DCPA (WSSA)
Other name(s): chlorthal-dimethyl (BIS, ISO); DAC 893; dimethyl tetrachloroterephthalate (IUPAC)
Trade name(s): DACTHAL®
Chemical family: phthalic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
DCPA



Molecular formula: $C_{10}H_6Cl_4O_4$
Molecular weight: 331.97 g/mole
Description: Off white or tan crystals, slightly aromatic
Density: NA
Melting point: 156 C
Boiling point: NA
Vapor pressure: 3.33×10^{-4} Pa (25 C)
Stability: Stable to UV light; decomposes at 360-370 C (differential thermal gravimetric analysis)
Solubility:
water 0.5 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 7.9 toluene 14.7
benzene 22 xylene 14
carbon tetrachloride 11.2

pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

DCPA can be applied as follows: PRE at 11.8-16.8 kg ai/ha in established turf or at 11.8 kg ai/ha in newly-seeded turf; PRE at 11.8-13.4 kg ai/ha in ornamentals; PRE at 5-11.8 kg ai/ha in Brassica spp. crops, beans, melons, cucumbers, squash, garlic, greens, horseradish, onions, potatoes, yams, tomatoes, eggplant, peppers, strawberries, and cotton. DCPA controls several annual broadleaf and grass weeds including crabgrass spp., annual bluegrass, creeping speedwell, and annual spurge spp. It can be applied in certain irrigation systems as well as by conventional sprayer.

USE PRECAUTIONS

Fire hazard: WP and WG formulation are nonflammable.
Corrosiveness: Non-corrosive
Storage stability: All formulated products are stable under normal storage conditions.
Cleaning glassware/spray equipment: Clean equipment with water
Incompatibilities: Compatible with most other pesticides; no unusual hard water problems.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits mitosis probably by affecting phragmoplast microtubule arrays and cell wall formation (1). (more details on page 12)
Symptomology: Following soil applications, susceptible seedlings typically do not emerge because DCPA inhibits germination and meristem growth.
Absorption/translocation: Not absorbed by foliage or translocated in the plant.
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Adsorbed by organic matter
K_{oc}: Average is 5000 mL/g (2)
Transformation:
Photodegradation: Negligible losses in the field
Other degradation: Microbial breakdown is the primary means of DCPA, dissipation from soil; rapidly hydrolyzed to the parent acid or diacid.
Persistence: Average field half-life is 60-100 d.
Mobility: Did not leach in any soils tested.
Volatilization: Negligible losses.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade DCPA unless otherwise indicated.

Acute toxicity:
Oral LD_{50} male rat, rabbit, and beagle dog, >10,000 mg/kg; Dermal LD_{50} rabbit, >10,000 mg/kg; 4-h inhalation LC_{50} rat, >5.7 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild
Subchronic toxicity: NA
Chronic toxicity:
24-mo dietary rat: NOEL NA; no effects at 10,000 mg/kg/d
24-mo dietary, dog: NOEL NA; no effects at 10,000 mg/kg/d
Teratogenicity:
Rabbit: NOEL NA; not teratogenic

Reproduction:

Rat: NOEL NA; no changes in fertility, gestation, live births, or lactation at 500 mg/kg/d

Mutagenicity:

Structural chromosome aberration: Cytogenetics, negative; Dormant lethal, negative

DNA damage/repair: Unspecified test, negative

Wildlife:

Bobwhite quail oral LD_{50}, ~1270 mg/kg; Honey bee, non-toxic.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: HP model 5711A with 0.125-in x 10-ft SS column, 5% XE-60 on 60-80 mesh Gas Chrom Z, column temperature of 215 C, detector temperature of 300 C, injection port temperature of 250 C, nitrogen as carrier gas regulated at 40 psig, flow rate of 33 mL/min, zero air regulated at 24 psig (about 200 mL/min), hydrogen regulated at 20 psig (set to give an air-hydrogen ratio of 6.7, about 30 mL/min), and chart speed of 0.25 in/min. Calculations are done by a Data System or by peak height measurement.

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Amvac

Reference(s):

1. Vaughan and Vaughan. 1990. Am. Bot. 65:379.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

desmedipham

CAS #: 13684-56-5 $5^{(C_1)}$

ethyl [3-[[(phenylamino)carbonyl]oxy]phenyl]carbamate

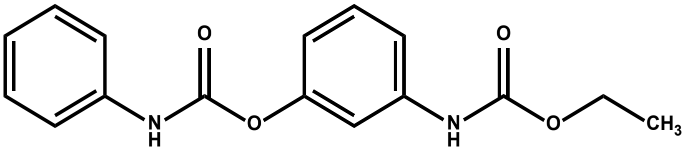
NOMENCLATURE

Common name: desmedipham (ANSI, BSI, ISO, WSSA)
Other name(s): desmediphame; EP-475; SN 38107; ZK 14,494; ethyl *m*-hydroxycarbanilate carbanilate (ester); ethyl 3-phenylcarbamoyloxycarbanilate (IUPAC); 3-ethoxycarbonylaminophenyl phenyl-carbamate
Trade name(s): BETANEX®; BETANEX® BETA; BETAMIX®; BETAMIX® BETA; BETANAL®; PROGRESS®; PROGRESS® BETA
Chemical family: carbanilate; phenylcarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

desmedipham



Molecular formula: $C_{16}H_{16}N_2O_4$
Molecular weight: 300.31 g/mole
Description: Colorless or light yellow crystalline solid
Density: NA
Melting point: 120 C
Boiling point: NA
Vapor pressure: 4×10^{-8} Pa (25 C)
Stability: NA
Solubility:
water ~7 mg/L (pH 7, 20 C)
organic solvents g/100 mL (20 C):
acetone ~40
benzene ~0.16
chloroform ~8
dibromoethane 1.78
n-hexane 0.05
methanol ~18
toluene 0.12
pK$_a$: None (non-ionizable)
K$_{ow}$: 2455 (pH 3.9)

HERBICIDAL USE

Desmedipham can be applied POST at 0.82-1.3 kg ai/ha in sugarbeets to control annual broadleaf weeds such as annual sowthistle, black nightshade, lambsquarters, common ragweed, and redroot pigweed.

USE PRECAUTIONS

Fire hazard: The product BETANEX is non-flammable; flash point is 68 C (TOC-ASTM D-1310)
Corrosiveness: Non-corrosive
Storage stability: BETANEX was stable for 4.5 mo during an accelerated storage test at 70 C
Cleaning glassware/spray equipment: Rinse equipment with water and detergent; rinse glassware with acetone
Emergency exposure: If ingested, induce vomiting or use gastric lavage
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Leaves appear water-soaked within a few days after application; chlorosis and necrosis follow soon thereafter
Absorption/translocation: Readily absorbed by foliage, but poorly translocated in the phloem to other plant parts (2). Rain falling within a few h of application may reduce efficacy.
Metabolism in plants: Hydrolysis of desmedipham to ethyl *N*-(3-hydroxyphenyl)carbamate and subsequently to *m*-aminophenol is one of the main pathways of metabolism in sugarbeets (3). The bacterial enzyme phenmedipham hydrolase, coded by a plasmid gene (*pcd*), catalyzed hydrolysis of the carbamate linkage of desmedipham (4).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: None known

BEHAVIOR IN SOIL

Sorption:
K$_{oc}$: Average is 1500 mL/g (5)
Transformation: NA
Persistence: Half-life <1 mo in silty loam, sandy loam, and silty clay loam soils
Mobility: No appreciable leaching; residues remain in the top 5 cm of soil
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade desmedipham unless otherwise indicated.

Acute toxicity:

Oral LD$_{50}$ rat, >10,250 mg/kg; mouse, >500 mg/kg; Dermal LD$_{50}$, NA; 4-h inhalation LC$_{50}$, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

BETANEX: Oral LD$_{50}$ rat, 3720 mg/kg; Dermal LD$_{50}$ rabbit, >2025 and <10,250 mg/kg

BETAMIX: Oral LD$_{50}$ rat, 4100 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg.

Subchronic toxicity: NA
Chronic toxicity:
18-mo dietary, mouse: NOEL 25 mg/kg/d
24-mo dietary, rat: NOEL ~3 mg/kg/d
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife:

Bobwhite quail 5-d dietary LC$_{50}$, >10,000 mg/kg; Mallard duck 5-d dietary LC$_{50}$, >10,000 mg/kg; Honey bee, non-toxic; Daphnia 48-h LC$_{50}$, 1.88 mg/L; Bluegill sunfish 96-h LC$_{50}$, 6 mg/L; Rainbow trout 96-h LC$_{50}$, 1.7 mg/L

BETANEX: Bobwhite quail oral LD$_{50}$, 2480 mg/kg;

Bluegill sunfish 96-h LC_{50}, 13.4 mg/L; Rainbow trout 96-h LC_{50}, 3.8 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Recrystallization

Analytical methods: Desmedipham can be separated from other compounds by TLC quantitative determination at 240 nm.

Historical: First reported in 1969 (1). U.S. patent 3,404,975. Schering Ag was issued Great Britain patent 1,127,050.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Arndt and Boroschewski. 1969. Symp. New Herbic. 3rd, p. 141.
2. Bromilow and Chamberlain. 1991. Pages 245 284 *in* R. C. Kirkwood, ed., Target Sites for Herbicide Action. Plenum Press, New York.
3. Knowles and Sonawane. 1972. Bull. Environ. Contam. Toxicol. 8:73.
4. Pohlenz, H. O. et al. 1992. J. Bacteriol. 174:6600.
5. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

desmetryn

CAS #: 1014-69-3 $5^{(C_1)}$

N-methyl-N′-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine

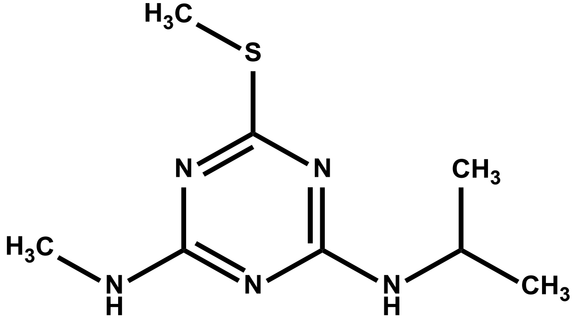
NOMENCLATURE

Common name: desmetryn (ISO)
Other name(s): demetryne; *N*^{2}-isopropyl-*N*^{4}-methyl-6-methylthio-1,3,5-triazine-2,4-diamine (IUPAC)
Trade name(s): SEMERON®
Chemical family: methythio triazine; methylthio-*s*-triazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

desmetryn



Molecular formula: $C_8H_{15}N_5S$
Molecular weight: 213.31 g/mole
Description: White crystalline solid
Density: 1.17 g/mole (20 C)
Melting point: 84-86 C
Boiling point: 345 C
Vapor pressure: 1.33 x 10^{-4} Pa (20 C)
Stability: No significant hydrolysis at 70 C detected at pH 5-13.
Solubility:
  water, 580 mg/L (20 C)
  readily soluble in most organic solvents
pK$_a$: 4.0 (weak base)
K$_{ow}$: log K_{ow} = 2.38

HERBICIDAL USE

Desmetryn is used for postemergence control of *Chenopodium album* and other broadleaf weeds and some grasses in most *Brassica spp.*, herbs, onions, leeks, and conifer seedbeds at rates of 0.25 to 0.5 kg a.i./ha. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Chlorosis followed by necrosis of affected plant tissue
Absorption/translocation: Absorbed by roots and leaves with translocation acropetally through the xylem; accumulates in the apical meristem
Metabolism in plants: Desmetryn is reported to be metabolized in plants by hydrolysis of the methylthio group followed by conjugation with glutathione and dealkylation
Mechanism of resistance in weeds: Altered target site

BEHAVIOR IN SOIL

Sorption:
  K$_{oc}$: 92-350 mL/g
Transformation:
  Photodegradation: NA
  Other degradation: Desmetryn undergoes microbial degradation to yield five products with the major metabolite being the 2-hydroxy product.
Persistence:
  Field experiments: DT_{50} 3 mo
  Lab experiments: DT_{50} 140 d
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade desmetryn unless otherwise indicated.

Acute toxicity:
  Oral LD_{50} rat, 1390 mg/kg; Dermal LD_{50} rabbit, >1000 mg/kg
Subchronic toxicity:
  90-d dietary, rat: NOEL 200 mg/kg/d
  90-d dietary, dog: NOEL 200 mg/kg/d
Wildlife:
  Japanese quail LC_{50} (8 d), >10000 mg/kg; Rainbow trout LC_{50} (96 h), 2.2 mg/L; common carp, 37 mg/L; Bees non-toxic LD_{50} (oral), >197 µg/bee; earthworms 14-d LC_{50}, 160 mg/kg soil; rat oral LD_{50}, 1390 mg/kg; mouse oral LD_{50}, 1790 mg/kg; rat dermal LD_{50}, 2000 mg/kg; rat inhalation LD_{50}, >1563 mg/kg; rat 90-d dietary, 20 mg/kg; dog 90 day dietary, 200 mg/kg
Use classification: WHO class III; EPA (formulation) III

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

dicamba

3,6-dichloro-2-methoxybenzoic acid

CAS # Acid: 1918-00-9
Dimethylammonium salt: 2300-66-5
Na salt: 1982-69-0

$4^{(O)}$

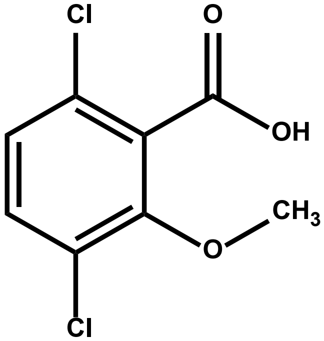
NOMENCLATURE

Common name: dicamba (ANSI, BSI, ISO, WSSA).
Other name(s): VEL-58-CS-11; 3,6-dichloro-2-methoxybenzoic acid (IUPAC); 3,6-dichloro-*o*-anisic acid (IUPAC)
Trade name(s): BANVEL®; BRASH®; CELEBRITY®; CELEBRITY® PLUS; CLARITY®; DISTINCT®; DYVEL®; DYVEL DSp; ENGENIA™; MARKSMAN®; NORTHSTAR®; ONETIME®; OVERDRIVE®; STATUS®; WEEDMASTER®; YUKON®
Chemical family: benzoic acid

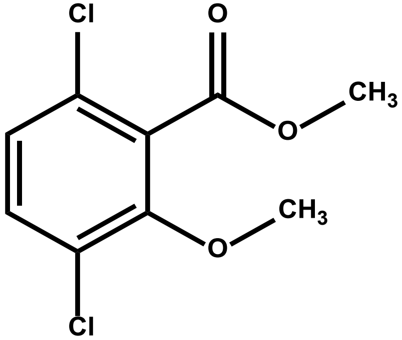
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

dicamba acid



Dicamba methyl



Molecular formula: *Acid* $C_8H_6Cl_2O_3$; *Diglycolamine (diolamine) salt* $C_{12}H_{17}Cl_2NO_5$; *Dimethylammonium (Dma) salt* $C_{10}H_{13}Cl_2NO_3$; *Na salt* $C_8H_5Cl_2NaO_3$*; N, N-Bis-(aminopropyl) methylamine salt* $C_{15}H_{25}Cl_2N_3O_3$
Molecular weight: *Acid* 221.04 g/mole; *Diglycolamine salt* 326.18 g/mole; *Dma salt* 266.12 g/mole; *Na salt* 243.02 g/mole
Description: Crystalline solid, white (reference grade) or brown (technical grade)
Density: 1.35-1.55 g/mL (25 C)
Melting point: 114-116 C
Boiling point: >200 C
Vapor pressure: 4.5 x 10^{-3} Pa (25 C)
Stability: Stable; resists oxidation and hydrolysis under normal conditions

Solubility:
Acid
water 4500 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 126
carbon disulfide 127
chloroform 51.6
cyclohexanone 91.6
diacetone alcohol 91
dichloromethane 26
dioxane 118
ethanol 92.2
n-hexane 0.375
methanol 137
methyl ethyl ketone soluble
1-octanol 68
pentane insoluble
tetrahydrofuran 139
toluene 13
xylene 20.2
heavy aromatic naphthane solvent 5.2
Dimethylamine salt
water 720,000 mg/L
pK_a: 1.87 (weak acid)
K_{ow}: 0.29

HERBICIDAL USE

Dicamba provides postemergence control of emerged weeds as well as moderate residual control of germinating weeds. Dicamba can be applied preplant and PRE at 0.56 kg ae/ha in corn, POST at 0.28 kg ae/ha in corn and sorghum, preharvest in sorghum at 0.28 kg ae/ha (Texas and Oklahoma only), POST at 0.07-0.14 kg ae/ha in small grains, POST at 0.28-2.24 kg ae/ha in pasture and rangeland, POST at 0.28-2.2 kg ae/ha in grasses and fallow, POST at 0.28-0.56 kg ae/ha in asparagus (California, Oregon, and Washington only), and POST at 0.28-1.1 kg ae/ha in turf. Dicamba is expected to be registered for PRE and POST applications in dicamba-tolerant cotton and soybean. Additional dicamba-tolerant crops are in development. Dicamba is also used for conservation reserve programs, grass grown for seed, sugarcane, turf, and noncropland sites. Many annual broadleaf weeds such as pigweed spp., wild buckwheat, and lambsquarters are controlled at 0.56 kg ae/ha, whereas certain perennial broadleaf weeds such as Canada thistle, perennial sowthistle, and field bindweed are controlled or suppressed at higher rates. To improve postemergence weed control, surfactants, crop oil concentrates, or sprayable fertilizers may be added. A spray system that delivers coarse droplet size is recommended to prevent off-target drift.

USE PRECAUTIONS

Fire hazard: Formulated products are non-flammable.
Corrosiveness: Formulated products are non-corrosive.
Storage stability: All formulated products are stable.
Cleaning glassware/spray equipment: Wash with detergent and rinse. Use acetone rinse for glassware
Emergency exposure: Flush eyes with water until clear; consult a doctor if irritation persists. Wash contaminated skin with mild soap and water and rinse; get medical attention if

skin irritation persists. If ingested, drink 1-2 glasses of water and induce vomiting.

Incompatibilities: Compatible with most herbicides and may be applied in liquid fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Similar to that of endogenous auxin (IAA) and other auxin-mimicking herbicides. (more details on page 12)

Symptomology: Symptoms include twisting and curling of stems and petioles (epinasty), stem swelling (particularly at nodes) and elongation, and leaf cupping. These symptoms are followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. At low application rates, the tips of new leaves may develop into narrow extensions of the midrib, and puckering of the young leaves may develop.

Absorption: Dicamba readily penetrates plant leaves, roots, and stems, but apparently not as rapidly as the phenoxyacetic acids such as 2,4-D (5). The dimethylamine formulation penetrates plant foliage more than other formulations (3). Dicamba transport across the plasmalemma may occur by passive diffusion as well as by an active, protein-mediated process (1) normally functioning in IAA transport.

Translocation: Dicamba is transported by both symplastic (including phloem) and apoplastic (including xylem) pathways and accumulates at the growing points. Translocation generally is slower in grasses and other tolerant species. Differential translocation among species has been associated with differential sensitivity. Dicamba translocates primarily apoplastically in wheat, but mostly symplastically in susceptible wild buckwheat (4). Following translocation to the roots, substantial percentages of dicamba exit into the surrounding medium (3).

Metabolism in plants: Dicamba metabolism generally is more rapid in tolerant species such as grasses than in susceptible broadleaf species (1). A number of metabolic reactions have been identified, including hydroxylation of dicamba to 5-hydroxy-2-methoxy-3-6-dichlorobenzoic acid, demethylation to salicylic acid derivatives, conjugation of dicamba or the demethylated and hydroxylated metabolites with glucose, and decarboxylation to unidentified metabolites.

Non-herbicidal biological properties: Auxin-like plant growth regulator.

Mechanism of resistance in weeds: A biotype of wild mustard from Western Canada is resistant to dicamba and other auxin herbicides. Although the mechanism of resistance has not been determined, resistance may be due to an insensitive target site (2). Populations of kochia in the U.S. Great Plains have also been documented as resistant to dicamba.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil

K_{oc}: Average is 2 mL/g (8)

Transformation:

Photodegradation: Dicamba is slowly photodegraded on soil under a xenon lamp, with a half-life equivalent to 269 d (40° N lattitude, springtime sunlight at noon). Thus, the contribution of photolysis to field dissipation likely is negligible (7).

Other degradation: Dicamba is metabolized to CO_2 in aerobic soil, with 3,6-dichlorosalicylic acid as the only major metabolite and low levels of 2,5-dihydroxy-3,6-dichlorosalicylic acid. Dicamba degrades more slowly in anaerobic soils. Non-biological degradation is negligible. At 52 and 95 wk after treatment with ^{14}C-dicamba, 18 and 3%, respectively, of the applied ^{14}C was unextractable.

Persistence: Studies and experience have shown that dicamba may be leached out of the zone of activity in humid regions in a period of 3-12 wk. Dicamba may persist significantly longer under conditions of low soil moisture and rainfall. Dicamba has a half-life of <14 d under conditions amenable to rapid metabolism.

Field experiments: Half-life of 4.4 d in a loam soil in Indiana.

Mobility: Low to medium leaching potential. Dicamba is mobile in soil but degrades rapidly. Low potential for runoff due to rapid degradation.

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dicamba acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1707 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >9.6 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, possible in sensitive individuals; Eye irritation rabbit, extreme

BANVEL: Oral LD_{50} rat, 2629 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.4 mg/L; Skin irritation rabbit, mild to moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, extreme

WEEDMASTER: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50} rat, >20.3 mg/L; Skin irritation rabbit, minimal; Eye irritation rabbit, minimal

Subchronic toxicity:

90-d dietary, rat: NOEL ~250 mg/kg/d (5000 mg/kg); decreased body weight and microscopic liver effects at 10,000 mg/kg

Chronic toxicity:

18-mo dietary, mouse: NOEL 115 mg/kg/d (1000 mg/kg); not oncogenic

24-mo dietary, rat: NOEL 125 mg/kg/d (2500 mg/kg); not oncogenic; no other effects

12-mo dietary, dog: NOEL 60 mg/kg/d (2500 mg/kg); no effects

Teratogenicity:

Rat: NOEL maternal 160 mg/kg/d, fetal 400 mg/kg/d; three pregnant dams treated with 400 mg/kg/d died on or before the second d and one non-gravid female died in this group; not teratogenic

Rabbit: NOEL maternal 30 mg/kg/d, fetal 300 mg/kg/d; abortions among females at 150 and 300 mg/kg/d were associated with maternal toxicity manifested as ataxia, weight loss, and reduced feed consumption; no effects on embryo/fetal viability or development at 300 mg/kg/d; not teratogenic.

Reproduction:

Rat: NOAEL 40 mg/kg/d (500 mg/kg); no effects on reproductive performance at up to 400 mg/kg/d (5000 mg/kg)

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: CHO, negative

DNA damage/repair: *B. subtilis*, positive

Wildlife:

Bobwhite quail oral LD_{50}, 216 mg/kg, 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck, oral LD_{50} 1373 mg/kg, 8-d dietary LC_{50}, >10,000 mg/kg; Daphnia 48-h TL_{50}, 110 mg/L; Bluegill sunfish 96-h TL_{50}, 135 mg/L; Rainbow trout 96-h TL_{50}, 135 mg/L; Sheepshead minnow 96-h TL_{50}, >180 mg/L; Fiddler crab 96-h TL_{50}, >180 mg/L

BANVEL: Bobwhite quail 8-d dietary LC_{50}, >4640 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg, 8-d dietary LC_{50}, >4640 mg/kg; Daphnia 48-h LC_{50}, 1600 mg/L; Bluegill sunfish 96-h LC_{50}, >1000 mg/L; Rainbow trout 96-h LC_{50}, 1000 mg/L

WEEDMASTER: Bobwhite quail 8-d dietary LC_{50}, >4640 mg/kg; Mallard duck oral LD_{50}, >4640 mg/kg, 8-d dietary LC_{50}, >4640 mg/kg; Daphnia 48-h LC_{50}, >1800 mg/L; Bluegill sunfish 96-h LC_{50}, >1000 mg/L; Rainbow trout 96-h LC_{50}, >1000 mg/L

Use classification: General use for most products. MARKSMAN is Restricted use because of groundwater contamination concerns with atrazine.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Residue analysis via extraction with aqueous acid and clean-up using SPE columns. Quantified by GLC of a suitable ester.

Historical: Invented by S. B. Richter. U.S. patent 3,013,054 was awarded in 1958.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Albaugh/Agri Star; Arysta; BASF; DuPont Crop Protection; Gowan; Helena; Loveland; Monsanto; Nufarm; PBI Gordon; Prokoz; Syngenta Crop Protection; Tenkoz; Winfield

Reference(s):

1. Ashton, F. M. and A. S. Crafts. 1981. Mode of Action of Herbicides, 2nd ed. Wiley-Interscience, New York.
2. Peniuk, M. G. et al. 1992. Abstr. Weed Sci. Soc. Am. 32:55.
3. Peterson, P. J. et al. 1985. Weed Sci. 33:717.
4. Quimby and Nalewaja. 1971. Weed Sci. 19:598.
5. Sargent, J. A. 1976. Pages 303-312 *in* L. J. Audus, ed., Herbicides: Physiology, Biochemistry, and Ecology. Academic Press, New York.
6. Scott and Norris. 1970. Nature 227:1366.
7. Sen, P. K. et al. 1993. Sandoz Agro, Inc., Lab Rep. No. 480065-23 (unpublished).
8. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
9. Klingaman, T. D. et al. 2012. North Central Weed Sci. Soc. Proc. p8.

dichlobenil

2,6-dichlorobenzonitrile

CAS #: 1194-65-6 **$20^{(L)}$**

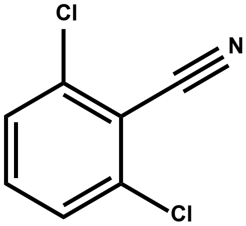
NOMENCLATURE

Common name: dichlobenil (ANSI, BSI, ISO, WSSA)
Other name(s): H-133
Trade name(s): ACME®; BARRIER®; DYCLOMEC®; NOROSAC®; CASORON®; CORSAGE®; FYDUTRIX®; DECABANE®; DU CASON; DO-DUSIT; DUDULEK G; FYDULAN®; FYDUMAS®; PREFIX™ D
Chemical family: benzonitrile;nitrile

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

dichlobenil



Molecular formula: $C_{17}H_3Cl_2N$
Molecular weight: 172.01 g/mole
Description: White to slightly yellow crystals, aromatic odor
Density: 0.6 g/mL
Melting point: 145-146 C (pure); 139-145 C (technical)
Boiling point: 270 C (1.0×10^5 Pa)
Vapor pressure: 7.33×10^{-2} Pa (20 C); 1.33×10^{-1} Pa (25 C); 2 Pa (50 C); 147 Pa (100 C)
Stability: Stable to sunlight and heat (at least 3 mo at 54 ± 1 C); stable at pH 5-9, but rapidly hydrolyzed by strong alkali to 2,6-dichlorobenzamide.
Solubility:

water (25 C), 20.5 mg/L (pH 5), 21.2 mg/L (pH 7), and 21.9 mg/L (pH 9)

organic solvents g/100 mL (20 C):

acetone 5 (8 C)	methylene chloride ~10
benzene ~5 (8 C)	toluene ~4
xylene 5.3 (25 C)	ethanol 1.5 (25 C)
cyclohexane 0.37 (25 C)	

pK_a: None (non-ionizable)
K_{ow}: 500

HERBICIDAL USE

Dichlobenil can be applied to the soil with or without incorporation in late fall or with incorporation in early spring as follows: at 4-8 kg ai/ha in fruit and nut orchards and nurseries; at 2.7-9 kg ai/ha in woody ornamentals, forests, and shelterbelts; at 4.5-8 kg ai/ha in vineyards; at 4.5 kg ai/ha in cranberries; at 11.2-22.4 kg ai/ha in nursery stock containers or noncrop areas for nutsedge control on mineral soils; at 11.2-13.4 kg ai/ha under asphalt; and at 7.3-22.4 kg ai/ha in industrial sites and other non-crop areas.

aquatic situations. Dichlobenil controls many annual and biennial broadleaf and grass weeds such as *Poa* spp., crabgrass spp., pineappleweed, purslane, Texas panicum, and wild carrot, as well as some perennial weeds including dandelion, Canada thistle, leafy spurge, quackgrass, and smooth brome.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-combustible.
Corrosiveness: Non-corrosive
Storage stability: Shelf life is >2 yr for technical and formulated products when stored cool and dry. Storage container should close tightly to prevent volatilization. Dichlobenil is stable to heat and largely stable to light.
Cleaning glassware/spray equipment: NA
Incompatibilities: Compatible with most WP- or WG-formulated herbicides. Mixing with liquid fertilizers or EC-formulated herbicides is not recommended.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Dichlobenil primarily inhibits actively-dividing meristems in the root and shoot as well as seed germination. It does not affect respiration or photosynthesis, but inhibits cellulose synthesis (1) (more details on page 15)
Symptomology: Following soil applications, susceptible seedlings typically do not emerge because dichlobenil inhibits germination and meristem growth.
Absorption/translocation: Readily absorbed by roots and leaves. Rapid acropetal translocation when root-absorbed, but slow basipetal translocation when absorbed by leaves.
Metabolism in plants: A percentage of root-absorbed dichlobenil is lost by evaporation from leaf surfaces. Dichlobenil is hydroxylated in plants, followed by conjugation.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to OM, but poorly to clay.

K_{oc}: Average is 400 mL/g (estimated) (2)

Transformation: Half-life was 10.2 d in water under simulated sunlight (equivalent to 40° north latitude). Losses in the field are low to negligible due to application as a granule

Other degradation: Metabolized by microbes to 2,6-dichlorobenzamide (BAM) and then via 2,6-dichlorobenzoic acid to carbon dioxide and other breakdown products. Non-biological degradation does not occur.

Persistence: Average field half-life is 60 d (2).
Labeled rates generally provide 2-6 mo weed control.

Field experiments: Half-lives as follows: 3.7 mo in a Colonic very fine loamy sand soil in New York;16 d in a sandy soil in California; 8 mo in a Woodburn silt loam in Oregon.

Lab experiments: Half-life is 1-6 mo depending on soil characteristics

Mobility: Low mobility; primary metabolite, BAM, is more highly leachable

Volatilization: Substantial losses when surface-applied to wet soil, especially with high temperatures; losses from dry soil are reduced by incorporation or application soon before rainfall or irrigation

Formulation effects: Granules reduce volatilization losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dichlobenil unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 4460 mg/kg; male mouse, 1014 mg/kg; female mouse, 1621 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; rat, >1000 mg/kg; 4-h inhalation LC_{50} rat, >0.25 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

CASORON G: Oral LD_{50} rat, >5000 mg/kg; mouse, >7500 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; Skin irritation rabbit, none; Eye irritation rabbit, none

CASORON 20G: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, moderate

CASORON G-4: Oral LD_{50} rat >5000 mg/kg; Skin irritation rabbit, none

CASORON 50W: Eye irritation rabbit, none.

Subchronic toxicity:

90-d dietary, mouse: NOEL 25 mg/kg/d

90-d dietary, rat: NOEL 2.5 mg/kg/d

90-d dietary, dog: NOEL 1.25 mg/kg/d

90-d dietary, hamster: NOEL 41 mg/kg/d

Chronic toxicity:

24-mo dietary, rat: NOEL 2.5 mg/kg/d; slight increase in benign liver tumors in female

12-mo dietary, dog: NOEL 1.25 mg/kg/d

24-mo dietary, dog: NOEL 1.25 mg/kg/d**20-mo dietary, hamster:** In Study 1, NOEL 10 mg/kg/d; not oncogenic. In Study 2, NOEL NA; slight increase in benign liver tumors in males

88-wk dietary, hamster: NOEL 132 mg/kg/d; not carcinogenic

Teratogenicity:

Rat: NOEL 180 mg/kg/d; not teratogenic

Rabbit: NOEL 45 mg/kg/d; malformations in the presence of maternal toxicity at 135 mg/kg/d

Mouse: NOEL 60 mg/kg/d; no effects; not teratogenic

Reproduction:

Rat: NOEL 3 mg/kg/d; no reproductive effects

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: *In vitro* and *in vivo* cytogenicity, negative; Mouse micronucleus, negative

DNA damage/repair: *In vitro* test, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, 5200 mg/kg; Japanese quail 8-d dietary LC_{50}, >5000 mg/kg; Pheasant 8-d dietary LC_{50}, 1500 mg/kg; Mallard duck oral LD_{50}, >50 mg/kg, 8-d dietary LC_{50}, >5200 mg/kg; Honey bee topical LD_{50}, >11 µg/bee; Daphnia 48-h LC_{50}, 6.2 mg/L; Bluegill sunfish 96-h LC_{50}, 6.72-8.31 mg/L; Fathead minnow 96-h LC_{50}, 6.3 mg/L; Rainbow trout 96-h LC_{50}, 4.93-6.26 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Single-step ammoxidation of 2,6-dichlorotoluene to 2,6-dichlorobenzonitrile

Purification of technical: Recrystallization from methanol and washing with water.

Analytical methods: Extract with dichloroethane, acetone, or acetonitrile. Samples are analyzed by GC using electron capture detection with a detection limit of 50 ppb. See Meulemans and Upton. J. AOAC 49:976-981.

Historical: Dichlobenil was discovered in the mid1950s at Philips-Duphar in The Netherlands. Biological properties were first described in 1960 (3); first marketed in The Netherlands in 1960. Dutch patent 97,486 and U.S. patent 3,027,248.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): PBI Gordon; Solvay Duphar; Uniroyal

Reference(s):

1. Hogetsu, T. et al. 1974. Plant Cell Physiol. 15:389.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1..
3. Koopman and Daams. 1960. Nature (London) 186:89

dichlormid

CAS #: 37764-25-3

NC

2,2-dichloro-N,N-di-2-propenylacetamide

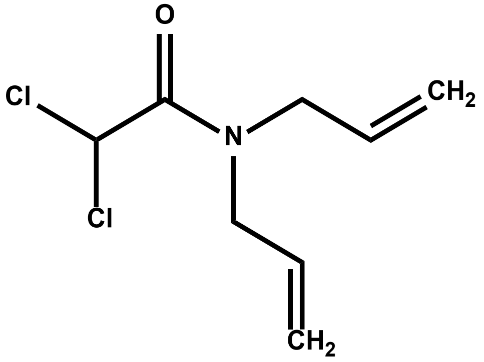
NOMENCLATURE

Common name: dichlormid (WSSA)
Other name(s): R-25788; *N*,*N*-diallyl-2,2-dichloroacetamide (IUPAC)
Trade name(s): **Note: R-29148 replaced dichlormid in ERADICANE 6.7-E, ERADICANE 25-G; ERADICANE 106; SURPASS®; SUTAN+ 6.7-E; SUTAZINE®
Chemical family: dichloroacetamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

dichlormid



Molecular formula: $C_8H_{11}Cl_2NO$
Molecular weight: 208.09 g/mole
Description: Clear liquid when pure, technical is clear amber to dark brown
Density: 1.195-1.2 g/mL (20 C)
Melting point: 5-6.5 C
Boiling point: 130 C (1.33 x 10^3 Pa)
Vapor pressure: 8.0 x 10^{-1} Pa (25 C); 1.33 Pa (50 C)
Stability: Slowly degraded by UV light (<10% after 30 d in water or on soil); Stable to hydrolysis in aqueous solution (25 C, pH 5, 7, or 9; 40 C, pH 5 or 7) half-life is 185 d (pH 9, 40 C)
Solubility:
  water 4388 mg/L (25 C)
  organic solvents g/100 mL (20 C):
  acetone miscible
  ethanol miscible
  kerosene 1.5
  xylene miscible
pK_a: None (non-ionizable)
K_{ow}: 69 ± 5 (25 C)

HERBICIDAL USE

Dichlormid is a herbicide safener (antidote) sold as a commercial package mixture with thiocarbamate and chloroacetamide herbicides for use in corn. Dichlormid is applied PRE or PPI at 0.14-0.45 kg ai/ha when applied as SURPASS EC, PRE or PPI at 0.14-0.29 kg ai/ha when applied as SURPASS 100, and PPI at 0.14-0.29 kg ai/ha when applied as SUTAZINE. Dichlormid protects corn from injury by acetochlor and butylate. The safener provides no weed control and does not protect weeds from control by acetochlor or butylate. In research experiments, dichlormid applied as a soil or seed treatment protects corn and milo from a variety of herbicides.

USE PRECAUTIONS

Fire hazard: Dichlormid technical is non-combustible; flash point is 149 C. During fire, formulated products may support combustion and may decompose violently to release toxic and flammable gases.
Corrosiveness: Formulated products can corrode steel, particularly in the presence of moisture.
Storage stability: Stable for several years of storage
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: Wash skin with soap and water; if irritation develops, get medical attention. Flush eyes with water for at least 15 min; if irritation develops, contact a physician. If ingested, drink 1-2 glasses of water but do not induce vomiting; seek medical attention.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Protects corn and sorghum from thiocarbamate and chloroacetamide herbicide injury by increasing the rate of herbicide detoxification by the plant. Dichlormid protected against metolachlor injury in sorghum and corn by inducing synthesis of glutathione *S*-transferase (GST) isozymes catalyzing conjugation of the herbicide with the tripeptide glutathione (4, 11). However, the mechanism by which dichlormid alleviates thiocarbamate injury seems less clear than for the acetanilides, and may involve more than one process. Dichlormid enhances sulfate metabolism, thereby elevating glutathione levels (1). Dichlormid-induced increases in GST activity correlated with thiocarbamate safening (9). Dichlormid protects corn against herbicide injury by inducing glutathione reductase activity in corn (8). Additional research (13) suggested that dichlormid may prevent inhibition of terpenoid biosynthesis by thiocarbamates and acetanilides. Dichlormid also synergized the activity of photosynthesis inhibiting herbicides in *Ipomoea* spp. This synergism was due to a reduction in levels of ascorbic acid which is known to protect plant tissues from photooxidative damage (6). Lastly, dichlormid has a chemical structure resembling EPTC and competitively inhibits EPTC uptake in corn cell cultures by a process that does not appear to require energy (5). This may contribute to its protective action when used with EPTC.
Symptomology: Dichlormid does not injure plants
Absorption/translocation: Readily taken up by corn roots and coleoptile and translocated throughout the plants via the apoplasm (including the xylem) (10). Experimental efficacy of dichlormid as a seed treatment suggests that it is absorbed through the seed coat.
Metabolism in plants: Dichlormid is rapidly metabolized

in corn to several metabolites and to CO_2. Apparently, a two-step oxidation occurs, displacing the chlorine atoms (by reaction with water) to form the glyoxylic acid amide derivative followed by oxidation to the oxamic acid analogue and then decomposition to CO_2.

Non-herbicidal biological properties: None known.

BEHAVIOR IN SOIL

Sorption: Some adsorption occurs

K_{oc}: Average is 40 mL/g (estimated) (2)

Transformation:

Photodegradation: Very little in water solutions

Other degradation: Primarily degraded by microbes

Persistence: Average field half-life is 7 d (2)

Lab experiments: Half-life was 7-8 d when incorporated into moist loam and loamy sand soils at 26.7 C.

Mobility: Dichlormid leached to a concentrated band at about half the depth of water movement in four different soils, although some of the antidote remained near the surface.

Volatilization: Rapidly lost when applied to moist soil surfaces and from aqueous solution.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dichlormid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 4450 mg/kg; female rat, 2275 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.5 mg/L; Skin irritation rabbit, mild-moderate; Skin sensitization guinea pig, yes (midsensitizer); Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, rat: NOEL 20 mg/kg/d

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife: NA

Use classification: SURPASS 100, SUTAZINE+, and SUTAZINE+ 18-6G are Restricted Use due to groundwater contamination concerns with atrazine. Other products are General Use.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Residues in plants and soil can be determined by solvent extraction followed by GC.

Historical: Discovered in 1970 as an antidote for preventing corn injury by EPTC. Antidotal activity of dichlormid was first reported in 1972 (3). Structure/activity studies with dichlormid analogues were reported in 1978 (10).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Adams, C. A. et al. 1983. Pestic. Biochem. Physiol. 19:350.
2. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
3. Chang, F. Y. et al. 1972. Can. J. Plant Sci. 52:707.
4. Dean, J. V. et al. 1990. Plant Physiol. 92:467.
5. Ezra, G. et al. 1982. Pestic. Biochem. Physiol. 18:107.
6. Fedtke and Strang. 1989. Z. Naturforsch. 45c:565.
7. Hatzios, K. K. 1983. Adv. Agron. 36:265.
8. Komives, T. et al. 1985. Proc. Br. Crop Prot. Conf.-Weeds, p. 1155.
9. Lay and Casida. 1976. Pestic. Biochem. Physiol. 6:442.
10. Lay and Niland. 1985. Pestic. Biochem. Physiol. 23:131.
11. Mozer, T. J. et al. 1983. Biochemistry 22:1068.
12. 12. Stephenson, G. R. 1978. J. Agric. Food Chem. 26:137.
13. Wilkinson, R. E. 1983. Pages 233-236 *in* J. Miyamoto and P. C. Kearney, eds., Pesticide Chemistry: Human Welfare and the Environment, Vol. 3. Pergamon, Oxford.

dichlorprop

2-(2,4-dichlorophenoxy)propanoic acid

CAS # Acid: 120-36-5

$4^{(O)}$

NOMENCLATURE

Common name: dichlorprop (BSI, ISO, WSSA); dichlorprop-P (*R*-isomer)

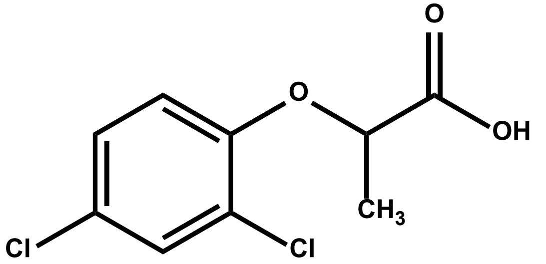
Other name(s): *dichlorprop* RD 406; 2,4-DP; (*RS*)-2-(2,4-dichlorophenoxy)propionic acid (IUPAC); 2-(2,4-dichlorophenoxy)propionic acid; (±)-2-(2,4-dichlorophenoxy)propionic acid; *dichlorprop-P* BAS 04418; (*R*)-2-(2,4-dichlorophenoxy)propionic acid

Trade name(s): BRUSH KILLER 2D + 2DP LOW VOL; CAREINE 2; CERTROL PA; CORNOX RK; DESORMONE; DISSOLVE®; DPD ESTER; DUPLOSAN DP; ENVERT® 171; HEDONAL; HEMOXONE; HERBITOX; KILDIP; MAYCLENE; POLYCLENE OPTICA DP®; WEEDONE®; REDIPON; SERITOX 50; STRIKE 3 ULTRA®; STRIKE 3 ULTRA® 2; 2,4-DP; TURF D + DP; TRIAMINE®; TRIESTER™; TRIESTER II; 2,4-DP; TANTIZON COMBI; TETROXONE M; VEGA; WINTERCORN EXTRA

Chemical family: phenoxy; phenoxyalkanoic acid; phenoxypropionic acid

CHEMICAL AND PHYSICAL PROPERTIES

dichlorprop acid



Dichlorprop butoxyethyl ester

Molecular formula: Acid $C_9H_8Cl_2O_3$; Butoxyethyl ester $C_{15}H_{20}Cl_2O_4$; Dimethylamine (Dma) salt $C_{11}H_{15}Cl_2NO_3$; Isooctyl ester (Io ester) $C_{17}H_{24}Cl_2O_3$

Molecular weight: Acid 235.07 g/mole; Be ester 335.23 g/mole; Dma salt 280.15 g/mole; Io ester 347.28 g/mole

Description: White to tan crystalline solid, faint phenolic odor

Density: ~1.42 g/mL

Melting point: 116-117.5 C

Boiling point: NA

Vapor pressure: 1 x 10^{-5} Pa (20 C)

Stability: NA

Solubility:

Acid

water 710 mg/L (28 C)

organic solvents g/100 mL (28 C):

acetone 59.5
benzene 8.5
ethanol 153
heptane 0.5
isopropanol 51
kerosene 0.21
toluene 6.9
xylene 5.1

Butoxyethyl ester

water 50 mg/L (estimated) (25 C) (2)

pK_a: 2.86 (weak acid)

K_{ow}: NA

HERBICIDAL USE

Dichlorprop can be applied as follows: in a spray-to-wet application at 443 g ae/100 L water for general brush control along fencerows, highways, and utility rights-of-way; directed spray-to-wet application at 1.77 kg/100 L water in pine plantations; POST at 12.4 kg ae/ha along railroad rights-of-way; POST at 8.3-12.4 kg ae/ha in utility rights-of-way; POST at 0.52-2.07 kg ae/ha for control of solid stands of oak or sandsage; POST at 4.14-10.4 kg ae/ha for general brush control along fencerows, highways, and utility rights-of-ways. Dichlorprop controls many hardwood and coniferous brush species.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: NA

Storage stability: NA

Cleaning glassware and spray equipment: NA

Emergency exposure: If ingested, induce vomiting

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood but similar to that of endogenous auxin (IAA) (more details on page 12)

Symptomology: Symptoms include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 3-5 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.

Absorption/translocation: NA

Metabolism in plants: NA

Non-herbicidal biological properties: NA

Mechanism of resistance in weeds: NA

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BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 1000 mL/g (estimated) for the butoxyethyl ester (2)

Transformation: NA

Persistence: Average field half-life is 10 d (2)

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dichlorprop acid unless otherwise indicated.**Acute toxicity:** Oral LD_{50} rat, 800 mg/kg, mouse, 400 mg/kg; Dermal LD_{50} mouse, 1400 mg/kg; 4-h inhalation LC_{50} NA; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation rabbit, none sensitization, NA; Eye irritation rabbit, none

Subchronic toxicity:

98-d dietary, rat: NOEL NA; not toxic at 12.4 mg/kg/d; slight liver hypertrophy at 50 mg/kg/d

Chronic toxicity:

90-d dietary, rat: NOEL NA; no effect at 12.4 mg/kg/d

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Dichlorprop butoxyethyl ester technical: Bluegill sunfish 96-h LC_{50}, 1.1 mg/L; Rainbow trout 96-h LC_{50}, 100-220 mg/L

Dichlorprop dimethylamine salt technical: Bluegill sunfish 96-h LC_{50}, 165 mg/L

Dichlorprop isooctyl ester technical: Bluegill sunfish 96-h LC_{50}, 16 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Produced by coupling 2-chloro-propionic acid with 2,4-dichlorophenol in alkaline solution. A slight molar excess of the phenol and a pH above 9 are needed for good coupling. The acid is obtained by adjusting pH to about 4.9-5.3 and extracting to remove unreacted DCP with toluene. Dichlorprop is then released by adding HCl.

Purification of technical: Recrystallize to improve color

Analytical methods: Analytical methods are the same as for 2,4-D with the necessary changes in equivalent weights in calculations.

Historical: Introduced as a herbicide commercially in 1961 by the Boots Co. Ltd.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Agriliance; Kwizda; Nufarm; UAP-Platte; Riverdale

Reference(s):

1. Tittle, F. L. et al. 1990. Plant Physiol. 94:1143.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

diclofop

2-[4-(2,4-dichlorophenoxy)phenoxy]propanoic acid

CAS # Acid: 40843-25-2
Methyl ester: 51338-27-3

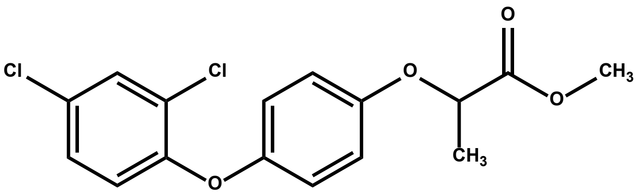
1$^{(A)}$

NOMENCLATURE

Common name: diclofop (ANSI, BSI, ISO, WSSA)
Other name(s): HOE-23408; (Acid) (RS)-2-[4-(2,4-dichlorophenoxy)phenoxy] propionoic acid (IUPAC); (Methyl ester) diclofop-methyl; methyl 2-[4-(2,4-dichlorophenoxy) phenoxy]propanoate; methyl (RS)-2-[4-(2,4-dichlorophenoxy)phenoxy]propionate (IUPAC)
Trade name(s): HOEGRASS® EC 500; HOELON®; ILLOXAN® 28; ILLOXAN® 36
Chemical family: aryloxyphenoxy

CHEMICAL AND PHYSICAL PROPERTIES

diclofop-methyl



Molecular formula**: Acid $C_{15}H_{12}Cl_2O_4$; Methyl Ester** $C_{16}H_{14}Cl_2O_4$
Molecular weight: Acid 327.16 g/mole Methyl Ester 341.19 g/mole
Description: Colorless, odorless crystals
Density: 1.3 g/mL (40 C)
Melting point: 39-41 C
Boiling point: 175-176 C (1.33 x 10^1 Pa)
Vapor pressure: 2.13 x 10^{-5} (25 C)
Stability: Degraded by UV light, strong acid, and strong alkali; decomposes at (~288 C)
Solubility:
Acid
water 3000 mg/L (22 C) Methyl Ester
water 0.8 mg/L
organic Solvents g/100 mL (20 C)
acetone 249 ethanol 11
diethyl ether 228 xylene 253
pK_a: Acid 3.57 (weak acid); Methyl Ester none (non-ionizable)
K_{ow}: 37,800

HERBICIDAL USE

Diclofop can be applied POST at 0.56-1.12 kg ai/ha in wheat, barely, Austrian winter pease, and lentils for control of certain annual grasses such as wild oats, foxtail, spp., barnyard grass, and annual ryegrass. Diclofop also can be applied PRE or PPI at 0.84-1.12 kg ai/ha in winter wheat for control of downy brome, ripgut brome, and other weeds, POST at 0.84-1.68 kg ai/ha in bermudagrass turf for goose grass control, and POST at 0.56-1.12 kg ai/ha in the Conservation Reserve program. Other tolerant crops include flax, sugar beets, and most broadleaf agronomic and horticultural crops.

USE PRECAUTIONS

Fire hazard: Technical methyl ester is slightly flammable; HOELON 3 EC is flammable; flash point is 26 ± 5 C by closed cup and 40 ± 5 C, by open cup
Corrosiveness: HOELON is non-corrosive
Storage stability: Stable for > 2 yrs; do not store below -7 C
Cleaning glassware/spray equipment: Wash glassware with water and detergent; wash equipment with detergent or an approved spray tank cleaner
Emergency exposure: If ingested, do not induce vomiting; seek immediate medical attention
Incompatibilities: Tank mixes with phenoxy herbicides such as 2,4-D and MCPA (especially amine formulations) antagonize grass control with diclofop.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details of page 12)
Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop 1-3 wk after application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Scattered chlorotic mottling may develop on some susceptible species and may resemble the burning that is characteristic of contact herbicides. With PRE applications, the first leaf may emerge, turn purple and die.
Absorption: The methyl ester is rapidly absorbed into roots or leaves. Diclofop acid is poorly absorbed into foliage. Diclofop ester and acid diffuse readily across the plasmalemma, although the acid form probably accumulates in cells by ion trapping typical of other weak acid herbicides (10). That is, the protonates acid diffuses across the membrane but the dissociated anion is excluded. Once inside the higher-pH environment of the cytoplasmic phloem cells, the protonated form of diclofop dissociates to the anion and is consequently trapped inside the cell because the anionic form can not diffuse through the non-polar membrane.
Translocation: Diclofop is systemic and is principally translocated in the phloem. Diclofop accumulates in the meristematic regions, but translocation out of treated leaves is slow and accounts for a low percentage of the amount absorbed.
Metabolism in plants: In both susceptible and tolerant grasses, the methyl ester of diclofop is rapidly hydrolyzed (demethylated) to the herbicidally-active diclofop acid. Wheat rapidly detoxifies the acid by producing at least three isomeric aryl-hydroxylated metabolites which are quickly conjugated to yield O-glycoside of diclofop (2, 9). Cytochrome

P450-dependent monooxygenases may catalyze the hydroxylation reactions leading to diclofop detoxification (6). Detoxification of applied diclofop occurs rapidly in plants, with only 20 and 10% diclofop acid remaining in oats and wheat, respectively, 24 h after treatment (8). In oat roots, diclofop acid was primarily conjugated at the carboxyl group to form a neutral glucose ester. This metabolite is not phytotoxic but can be readily hydrolyzed to yield herbicidally active diclofop acid. As such, the glucose ester is not a true detoxification metabolite and its production does not protect oats from diclofop phytotoxicity.

Non-herbicidal biological properties: No fungicide, nematicide, or insecticide activity has been noted.

Mechanism of resistance in weeds: Resistance in biotypes of normally sensitive grass weeds, including Lolium multiforum, has been associated with an insensitive site of action. However, in rigid rygrass (L. rigidum) from Australian, cross-resistance to a number of herbicides including diclofop is not due to reduced ACCase sensitivity, but may be conferred by increased diclofop metabolism (7) or by sequestration away from the site of action. A biotype of wild oats from Canada recently was reported to be resistant to diclofop (3), but no mechanism has yet been determined.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 16000 mL/g for the methyl ester (11).

Transformation: Hydrolyzed within a few d under aerobic conditions to the herbicidally-active diclofop acid which then is metabolized with a half-life of 10 d in sandy soils and ~30 d in sandy clay soils. Small amounts of 4-(2,4-dichlorophenoxy)phenol also are produced. Under anaerobic conditions, results were similar except that ester hydrolysis to yield the acid was extremely rapid (within 1 h), and after 2 d up to 86% of applied diclofop was metabolized to various metabolites of diclofop acid while up to 3.7% was found as phenol metabolities.

Persistence: Average field half-life of the parent acid is 30 d at pH 7

Mobility: Little leaching potential

Volatilization: NA

Effects on soil microbes: In a sandy loam from Oregon and a loam from Indiana, 1 µg/g diclofop showed no bactericidal or fungicidal effects under aerobic or anaerobic conditions; rates of nitrogen fixation, nitrification utilization of cellulose, starch, and protein were not altered by microbes

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade diclofop methyl ester unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 557-580 mg/kg, dog, >1600 mg/kg; Dermal LD_{50} rat, >5000 mg/kg, rabbit 180 mg/kg; 4-h inhalation LC_{50} rat, >38.83 mg/L; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation rabbit, none

HOELON 3EC: Oral LD_{50} rat, 2020-2176 mg/kg; Dermal LD_{50} rat, >5000 mg/kg, rabbit 640 mg/kg; 4-h inhalation, 8.274 mg/L; Skin irritation, rabbit, slight

Subchronic toxicity: NA

Chronic toxicity:

24-mo dietary, rat: NOEL 20 mg/kg/d

15-mo dietary, dog: NOEL 8 mg/kg/d

Teratogenicity: NA

Reproduction:

Rat: NOEL >30 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Mouse micronucleus, negative; dominant lethal, negative

Wildlife:

Bobwhite quail oral LD_{50}, 4400 mg/kg; 8-d dietary LC_{50},13,000 mg/L; Japanese quail oral LD_{50}, >10,000 mg/kg; Coturnix quail 8-d dietary LC_{50}, >20,000 mg/kg; Mallard duck 8-d dietary LD_{50}, >20,000 mg/kg; Honey bee non-toxic; Rainbow trout 96-h LC_{50}, 0.35 mg/L

HOELON 3EC: Honey bee, non-toxic; Daphnia 48-h LC_{50}, 4.03 mg/L; Carp 96-h LC_{50}, 2.6mg/L; Rainbow trout 96-h LC_{50} , 1.38 mg/L

Use classification: Restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical Methods: The following method allows detection of diclofop methyl ester, diclofop acid, and the 5-hydroxy acid [2-[4-(2,4- dichloro-5-hydroxy phenoxy)phenoxy]propanic acid], and the phenol metabolite [4-(2,4-dichloro-phenoxy) phenol] on plants and soil. Hydrolysis of residues to the free carboxylic acids by refluxing in 1 N NaOH. This preparation is cleaned up by extractions, the acidified and methylated to form methyl ester derivatives (ring-hydroxylated metabolites will be converted to the ring-methoxy form, and phenol metabolites to the methoxy ether (anisol) form). The samples are further cleaned up with Florisil/Alumina column chromatography followed by chromatography through a SEP-PACK C^{18} (Waters Assoc., Milford, MA). Detection is done by GC with an electron capture detector. The severe hydrolytic procedure frees diclofop methyl ester from all the above-noted matrices, but does not otherwise alter their structure. Detection limit is 50 ppb.Historical: Herbicidal activity of diclofop was reported in 1975 (5).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Burton, J. D. et al. 1989. Pestic. Biochem. Physiol. 34:76.
2. Jacobson and Shimbabukaro. 1984. J. Agric. Food Chem. 32:742.
3. Joseph, O.O. et al. 1990. Weed Sci. 38:475
4. Kobek, K. et al. 1987 Z. Naturforsch. 43c-47.
5. Langeluddeke, O. et al. 1975. Mitt. Biol. Bundesanst. Land.-Forrstwirtsch. Berlin-Dahlem. 165:169.
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7. Powles, S. B. et al. 1990. Pages 394-406 in M.B. Green , H.M. LeBaron, and W. K. Moberg, eds.,

Managing Resistance to Agrochemicals. Am. Chem. Soc. Symp. Ser. 421, Washington DC.

8. Shimabukuro, R.H. et al. 1979. J. Agric. Food Chem. 27:615
9. Shimabukuro, R.H. et al. 1987. J. Agric. Food Chem. 35:393
10. Tritter, S.A. et al. 1987. Can. J. Plant Sci. 67:215.
11. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

diclosulam

CAS #: 145701-21-9

$2^{(B)}$

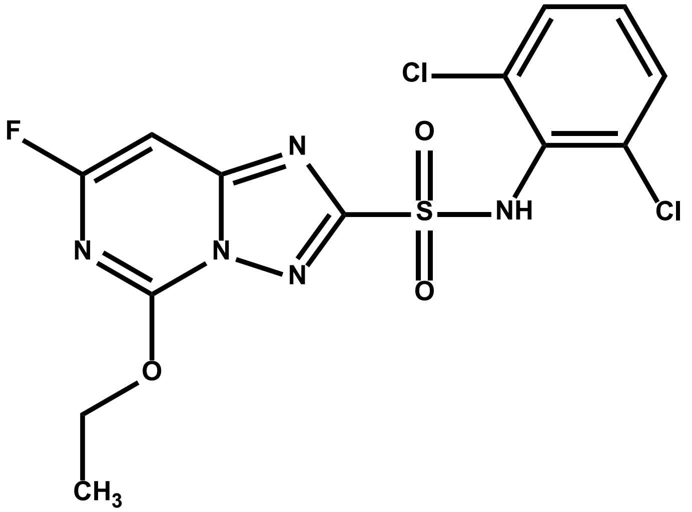
N-(2,6-dichlorophenyl)-5-ethoxy-7-fluoro[1,2,4] triazolo[1,5-*c*]pyrimidine-2-sulfonamide

NOMENCLATURE

Common name: diclosulam (BSI, pa ISO, ANSI, WSSA)
Other name(s): XDE-564; 2',6'-dichloro-5-ethoxy-7-fluoro[1,2,4]triazolo[1,5-*c*]pyrimidine-2-sulfonanilide (IUPAC)
Trade name(s): STRONGARM®
Chemical family: triazolopyrimidine sulfonamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *diclosulam*



Molecular formula: $C_{13}H_{10}Cl_2FN_5O_3S$
Molecular weight: 406.22 g/mole
Description: Off-white solid
Density: 1.60 g/mL (20 C)
Melting point: 218-221 C
Vapor pressure: 6.58×10^{-8} Pa (25 C)
Stability: Found to be stable after 28 d at 50 C alone and with stainless steel, mild steel, brass and in the presences of metal ions**Solubility:**

water, 117 mg/L (pH 5, 20 C); 124 mg/L (pH 7, 20 C); 4290 mg/L (pH 9, 20 C)
solvents (20 C) in g/100mL
acetone 0.797
acetonitrile 0.459
dicloromethane 0.217
ethyl acetate 0.145
methanol 0.0813
octanol 0.00442
toluene 0.00588

pK_a: 4.09 (20 C) (weak acid)
K_{ow}: log K_{ow}1.42 (pH 5); -0.047 (pH 7); -0.448 (pH 9)

HERBICIDAL USE

Diclosulam is a soil-applied herbicide for broadleaf weed and perennial nutsedge control in peanuts. It can be applied preemergence, preplant surface, and preplant incorporated. Application rate for peanuts is 26 g ai/ha.

USE PRECAUTIONS

Fire hazard: The product STRONGARM is dry and non-combustible.
Storage stability: Stable at normal temperatures and storage conditions.
Emergency exposure: Wash skin with soap and water, if irritation develops seek medical attention. Irrigate eyes with water for at least 15 min and seek medical attention. If swallowed, seek medical attention. Do not induce vomiting unless directed to do so by medical personnel.
Irritant: May cause pain and moderate eye irritation
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: After soil-applied treatment with diclosulam, broadleaf weeds fail to emerge or emerge but die quickly.
Absorption/translocation: Roots, and to a lesser extent shoots, of germinating seedlings intercept the compound as they grow and expand through the soil. Exposure to diclosulam may prevent sensitive weed seedlings from emerging, or weed seedlings may emerge but not develop beyond the cotyledon stage before expressing diclosulam symptomology. Weeds that do emerge through a diclosulam treatment continue to absorb and distribute the compound throughout the plant. Evaporation at leaf surfaces rapidly pulls water and solutes, including diclosulam, from the roots toward the shoot where toxic amounts finally accumulate in growing points and leaf tips. As it travels, some of the absorbed compound moving through the xylem and phloem diffused into surrounding tissues and does not reach these target areas.
Metabolism in plants: Research indicated that soybeans and peanuts exhibit limited translocation of diclosulam, and can quickly metabolize it into a non-active form. Specifically, soybeans have been shown to metabolize half of the diclosulam treatment in 3 hours. As a result of this rapid metabolism and limited translocation, soybeans and peanuts have a high tolerance to soil-applied diclosulam.
Non-herbicidal biological properties: None known

BEHAVIOR IN SOIL

Sorption: Soil moisture and soil organic matter have the greatest impact on diclosulam adsorption. Unlike some other sulfonamides, soil pH has minimal effect on the adsorption of diclosulam.

K_d: Range 0.6 to 3.8 L/kg, indicating relatively weak adsorptivity.

Transformation:

Photodegradation: Not an important route of dissipation.

Persistence:

Aerobic soil metabolism: Microbial metabolism is the primary degradation mechanism in soil. Laboratory first order half-lives ranged from 33 to 65 days.

Field Dissipation:

First-order half-lives ranged from 22 to 43 days. These half-lives are shorter than found for the same soils in the aerobic soil metabolism studies since additional degradation processes, including photolysis, are present under field conditions. As seen with the laboratory soil metabolism studies, initial degradation was rapid compared to later time points (biphasic degradation).

The total time required for diclosulam to reach the no effect level for plants is dependent upon plant sensitivity and the original application rate.

Mobility: Although diclosulam is mobile in soil, it has a low use rate which ranges from 20 to 42 g a.i. /ha. This low use rate, coupled with a typical 33 to 65 day half-life, means diclosulam is not likely to contaminate groundwater.

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade diclosulam unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Inhalation LC_{50} rat, >5.04 mg/L; Eye irritation in rabbit, very slight - resolved within 48 hr; Dermal irritation in rabbit, none; Dermal sensitization in guinea pig, none. Neurotoxicity NOEL > 2000 mg/kg bw/day

STRONGARM: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg. Inhalation LC_{50} rabbit, >6.70 mg/L; Eye irritation in rabbit, slight-to-moderate – resolved within 7 d; Dermal irritation in rabbit, slight – resolved within 7 d; Dermal sensitization in guinea pig, none

Subchronic toxicity:

90-d dietary, mouse: NOEL 100 mg/kg/d

90-d dietary, rat: NOAEL 50 mg/kg;.

90-d dietary, dog: NOEL 5 mg/kg/d

Chronic toxicity:

24-mo dietary, mouse: NOAEL 50 mg/kg/d male NOEL 50 mg/kg/d female (not oncogenic)

24-mo dietary, rat: NOEL 5 mg/kg/d (not oncogenic)

12-mo dietary, dog: NOEL 25 mg/kg/d

Teratogenicity:

Rat: NOEL 1000 mg/kg/d; not teratogenic

Rabbit: NOEL 65 mg/kg/d (maternal); NOEL 650 mg/kg/d (embryo/fetal)

Reproduction:

Rat: NOEL 1000 mg/kg/d; not reproductive toxin.

Mutagenicity:

Gene mutation: Ames test, negative

DNA damage/repair: ***in vitro*** Chromosomal aberrations negative

in vitro CHO-HGPRT, negative

in vivo mouse micronucleus, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck dietary LC_{50}, >5620 mg/kg; Rainbow trout 96-h acute LC_{50}, >110 mg/L; Bluegill 96-h acute LC_{50}, >137 mg/L; Sheepshead minnow 96-h acute LC_{50}, >120 mg/L; Daphnia, 48-h acute LC_{50}, 72 mg/L, EC_{50}, 55 mg/L; Grass shrimp 96-h acute LC_{50}, >120 mg/L; Eastern Oyster 96-h acute EC_{50}, >120 mg/L; Honeybee, 48-h acute contact LC_{50}, >25 ug/bee; Earthworms 14-d acute LC_{50}, >991 mg/kg; *Lemna gibba* 14-d acute EC_{50}, 1.24 µg/L; *Selenastrum capricornutum* 5-d acute EC_{50}, 1.7 µg/L; *Skeletonema costatum* (marine diatom), 5-d acute EC_{50}, >113 mg/L; *Navicula pelliculosa* (freshwater diatom), 5-d acute EC_{50}, >46 mg/L; *Anabaena flos-aquae* (blue-green algae) 5-d acute EC_{50}, 83 µg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical:

Developed by DowElanco. Registered by Dow AgroSciences in 2000.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

diethoLATE

CAS #: 32345-29-2 **NC**

O,*O*-diethyl *O*-phenyl phosphorothioate

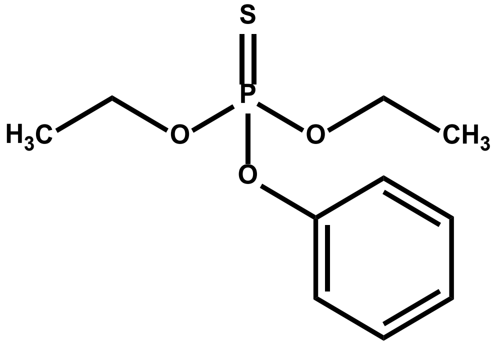
NOMENCLATURE

Common name: diethoLATE (WSSA)
Other name(s): R-33865; *O*,*O*-diethyl *O*-phenyl phosphorothioate (IUPAC)
Trade name(s): ERADICANE EXTRA®
Chemical family: None generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

diethoLATE



Molecular formula: $C_{10}H_{15}O_3PS$
Molecular weight: 246.26 g/mole
Description: Technical is a clear amber liquid
Density: 1.150 g/mL (20 C)
Melting point: Pour point (< -60 C)
Boiling point: 150 C (1.33 x 10^3 Pa)
Vapor pressure: 1.03 Pa (40 C)
Stability: NA
Solubility:
water 22 mg/L (25 C)
organic solvents (25 C):
miscible in acetone chlorobenzene
ethanol kerosene
xylene
pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

DiethoLATE is a non-phytotoxic microbial inhibitor sold in a commercial package mixture with EPTC or butylate for use on corn. By inhibiting soil microbes that degrade EPTC and butylate, diethoLATE extends the soil residual life of these herbicides and thereby increases the duration of weed control efficacy. As such, diethoLATE often is referred to as a herbicide extender. DiethoLATE is applied PPI at 0.75-1.12 kg ai/ha.

USE PRECAUTIONS

Fire hazard: Exothermic decomposition generating toxic and flammable gases may occur during fires or at temperatures above 200 C.
Corrosiveness: Corrosive to aluminum (<0.1 mg/cm²/yr), carbon steel (0.6 mg/cm²/yr), #304 stainless steel (0.1 mg/cm²/yr), and #316 stainless steel (0.1 mg/cm²/yr).
Storage stability: Discoloration can occur if stored in containers of mild steel. Use glass-lined steel or stainless steel containers.
Cleaning glassware/spray equipment: Clean glassware with acetone followed by water; flush equipment with water
Incompatibilities: DiethoLATE is relatively non-reactive, but does react with oxidizing agents.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits growth of soil microbes that degrade EPTC and butylate in soil.
Symptomology: DiethoLATE does not injure plants.
Absorption/translocation: DiethoLATE is not normally applied to foliage, but may be absorbed by the leaves from spray and vapors.
Metabolism in plants: NA
Other biological properties: None known

BEHAVIOR IN SOIL

Sorption: NA
Transformation: <2% of soil-applied diethoLATE was degraded in sterile soil in 60 d, but up to 26% of ring-labeled diethoLATE was metabolized to $^{14}CO_2$ in non-sterile soil under the same conditions. Bound residues were <10% of the applied.
Persistence: Not expected to persist in soil
Lab experiments: Half-life was 2-4 wk
Mobility: NA
Volatilization: 24% of soil-applied diethoLATE was lost after 2 wk at 28 C.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade diethoLATE unless otherwise indicated.
Acute toxicity:
Oral LD_{50} male rat, 681 mg/kg; female rat, 501 mg/kg; Dermal LD_{50} rabbit, 4640 mg/kg; 4-h inhalation LC_{50} male rat, 3.5 mg/L; female rat, 2.7 mg/L; Skin irritation rabbit, mild; Skin sensitization, NA; Eye irritation, NA
Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Cedar

difenzoquat

1,2-dimethyl-3,5-diphenyl-1*H*-pyrazolium

CAS # Cation: 49866-87-7
Methyl sulfate salt: 43222-48-6

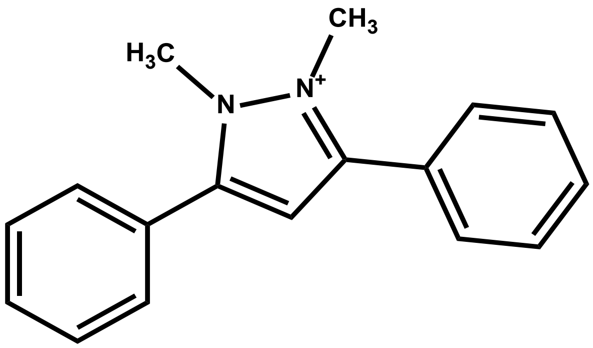
26$^{(Z)}$

NOMENCLATURE

Common name: difenzoquat (ANSI, BSI, ISO, WSSA)
Other name(s): AC 84,777; CL 84,777; 1,2-dimethyl-3,5-diphenylpyrazolium (IUPAC)
Trade name(s): AVENGE®
Chemical family: pyrazole, quaternary ammonium

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
difenzoquat cation



Difenzoquat

Molecular formula: *Cation:* $C_{17}H_{17}N_2$;
Methyl sulfate salt: $C_{18}H_{20}N_2O_4S$
Molecular weight: *Cation:* 249.34 g/mole;
Methyl sulfate salt: 360.43 g/mole
Description: White to off-white crystalline solid, odorless
Density: 0.796 g/mL (25 C)
Melting point: 156.5-158 C (with decomposition)
Boiling point: NA
Vapor pressure: 1 x 10^{-4} Pa (25 C)
Stability: Stable to light and heat; no loss after 3 mo at 45 C or after 169 h at 120 C; decomposes at >227 C; stable in acid; unstable in alkaline conditions
Solubility:
water 817,000 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 0.975
chlorobenzene 0.04
chloroform 500 (20 C)
ethylene dichloride 7.12
isopropanol 0.07
kerosene insoluble
methanol 58.8
xylene <0.01
pK_a: NA
K_{ow}: log K_{ow} = 4.45 (pH 5); 1.2 (pH 6); 0.238 (pH 7), 0.374 (pH 8); 0.479 (pH 9)

HERBICIDAL USE

Difenzoquat can be applied POST at 0.7-1.12 kg ae/ha in barley and wheat for wild oat control. Certain hard red spring wheat cultivars are susceptible. Non-ionic surfactant is required for maximum efficacy when spray water volumes exceed 94 L/ha.

USE PRECAUTIONS

Fire hazard: Technical is dry and non-flammable. AVENGE is non-flammable; flash point is >82 C (TOC).
Corrosiveness: AVENGE in aqueous solution may corrode tinplate, zinc, and aluminum, but not 316 stainless steel.
Storage stability: Shelf life of AVENGE is 2 yr
Cleaning glassware/spray equipment: Wash with water and detergent
Emergency exposure: Wash skin with soap and water. Corrosive to eyes, causing irreversible damage. If ingested, drink large quantities of milk, egg white, gelatin solution, or if these are not available, water. Probable mucosal damage may contraindicate use of gastric lavage.
Incompatibilities: AVENGE is compatible for tank mixing with broadleaf herbicides such as MCPA amine and ester, bromoxynil, MCPA plus bromoxynil, 2,4-D amine and ester, chlorsulfuron, and metsulfuron. AVENGE also can be mixed with fungicides such as benomyl, carbendazim, ethirimol, thiophanate methyl, tridemorph, and maneb/carbendazim mixtures, with the plant growth regulator, CYCOCEL, and with foliar fertilizer. Hydrogen may be generated if AVENGE solutions contact aluminum.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Effects include inhibition of nucleic acid biosynthesis (4), photosynthesis and ATP production (2), K+ absorption, and P incorporation into phospholipids and DNA. (more detail on page 15)
Symptomology: Plant growth ceases soon after application, and injury symptoms appear after 3-7 d. Meristematic areas become chlorotic, followed by general foliar chlorosis and necrosis.
Absorption/translocation: Absorbed rapidly into foliage following POST application. Translocation is primarily in the xylem and consequently is very limited following foliar absorption (5).
Metabolism in plants: Susceptible and tolerant plants apparently do not metabolize difenzoquat appreciably. Spring wheat tolerance correlates with a single dominant gene and modifier genes (1).
Non-herbicidal biological properties: Fungicidal activity against powdery mildew
Mechanism of resistance in weeds: Several resistant wild oat biotypes selected by use of triallate in Montana and Alberta are also resistant to difenzoquat (3). Mechanism of resistance is unknown.

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to clay particles due to its cationic nature.
K_{oc}: Average is 54,500 mL/g (6)
Transformation:
Photodegradation: Negligible losses

Other degradation: Not appreciably degraded by microbes

Persistence: Average half-life is <4 wk

Mobility: Negligible due to strong adsorption to clay; field studies do not indicate any potential for difenzoquat to move

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade difenzoquat methyl sulfate salt unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 617 mg/kg; female rat, 373 mg/kg; male mouse, 31 mg/kg; female mouse, 44 mg/kg; male rabbit, 470 mg/kg; Dermal LD_{50} male rabbit, >2000 mg/kg; 4-h inhalation LC_{50}, 0.5 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, corrosive (irreversible)

AVENGE: Oral LD_{50} male rat, 863 mg/kg; female rat, 912 mg/kg; Dermal LD_{50} rabbit, >2028 mg/kg; 4-h inhalation LC_{50} rat, >410.5 mg/L; Skin irritation rabbit, mild; Eye irritation rabbit, corrosive (irreversible)

Subchronic toxicity:

90-d dietary, rat: NOEL 250 mg/kg/d (2500 mg/kg)

90-d dietary, dog: NOEL 12.5 mg/kg/d (500 mg/kg)

Chronic toxicity:

18-mo dietary, mouse: NOEL 75 mg/kg/d (500 mg/kg); not oncogenic

24-mo dietary, rat: NOEL 25 mg/kg/d (500 mg/kg); not oncogenic

Teratogenicity:

Rat: NOEL >2500 mg/kg/d; no teratogenic or fetotoxic effects

Rabbit: NOEL maternal 100 mg/kg/d, developmental 250 mg/kg/d; decrease in maternal survival rate at maximum dose (250 mg/kg/d)

Reproduction:

Rat: NOEL 25 mg/kg/d (500 mg/kg) in a 3-yr study

Mutagenicity:

Gene mutation: CHO/HGPRT, negative

Structural chromosome aberration: CHO, negative

DNA damage/repair: Rat hepatocytes, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >4640 mg/kg; Mallard duck 8-d dietary LC_{50}, 10,388 mg/kg; Honey bee topical LD_{50}, >36.3 µg/bee; Bluegill sunfish 96-h LC_{50}, 696 mg/L; Rainbow trout 96-h LC_{50}, 694 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Difenzoquat is extracted from foliage and straw with methanol and from grain with chloroform. After removal of many coextractives by solvent partitionings, final clean-up is achieved by alumina column chromatography. Difenzoquat concentration is measured by GLC using a nitrogen-sensitive detector and the external standardization technique. The methods have a validated sensitivity limit of 0.1 mg/kg in foliage and straw and 0.05 mg/kg in grain.

Historical: Herbicidal properties of difenzoquat metilsulfate (the methyl sulfate) were first reported in 1973 (7). U. S. registration was obtained by American Cyanamid in 1975. U. S. patents 3,882,142 and 3,922,161 were awarded to American Cyanamid.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): AMVAC

Reference(s):

1. Busch, R. et al. 1989. Crop Sci. 29:47.
2. Halling and Behrens. 1983. Weed Sci. 31:693.
3. O’Donovan, J. T. et al. 1994. Weed Sci. 42:195.
4. Pallet and Caseley. 1980. Pestic. Biochem. Physiol. 14:144.
5. Sharma, M. P. et al. 1976. Weed Sci. 24:379.
6. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
7. Weis, M. E. et al. 1973. Proc. North Cent. Weed Control Conf. 28:100.

diflufenican

CAS #: 83164-33-4 **$12^{(F_1)}$**

N-(2,4-difluorophenyl)-2-[3-(trifluoromethyl)phenoxy]-3-pyridinecarboxamide

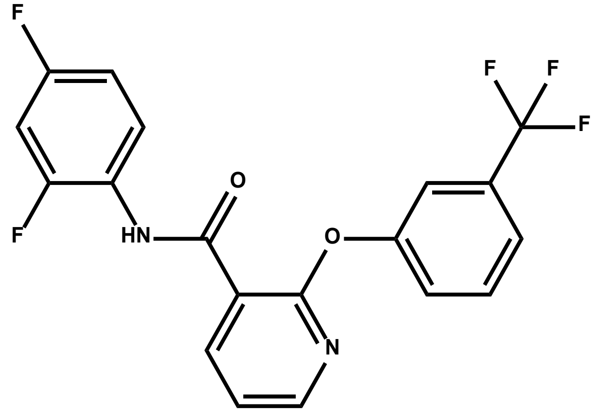
NOMENCLATURE

Common name: diflufenican (ISO published)
Other name(s): diflufenicanil; 2',4'-difluoro-2-(α, α, α-trifluoro-*m*-tolyloxy)nicotinanilide (IUPAC)
Trade name(s): BACARA®; BRODAL®; CARAT®; COUGAR; GALACE®; HERALD®; INGOT®; JAVELIN;
Chemical family: anilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

diflufenican



Molecular formula: $C_{19}H_{11}F_5N_2O_2$
Molecular weight: 394.3 g/mole
Description: Colorless crystals
Density: 1.19 g/mL
Melting point: 159-161 C
Boiling point: **>**100 C
Vapor pressure: 4.25 x 10^{-6} Pa (25 C)
Stability: Stable in air up to melting point
Solubility:
water <0.05 mg/L (25 C)
soluble in most organic solvents
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 4.9

HERBICIDAL USE

Diflufenican is used preemergence or early postemergence in autumn sown wheat and barley to control grass and broadleaved weeds, particularly *Gallium, Veronica* and *Viola* spp. Normally used in combination with isoproturon or other cereal herbicides.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: Non-corrosive
Storage stability: Stable under normal storage conditions.
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme phytoene desaturase in the carotenoid biosynthesis pathway (more details on page 14)
Symptomology: Sensitive plants cease growing over days develop symptoms including stunting, discoloration and necrosis which finally result in death of the weeds.
Absorption/translocation: Absorption principally by the shoots of germinating seedlings, with limited translocation.
Metabolism in plants: In cereals, rapidly meta-bolized via the nicotinamide and nicotinic acid to CO_2.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 1622 – 2369 mL/g
Transformation*:* Degradation proceeds via the metabolites 2-(3-trifluoromethylphenoxy) nicotinamide and 2-(3-trifluoromethylphenoxy) nicotinic acid to bound residues and CO_2.
Persistence: Field dissipation DT_{50} = 15-30 wks
Mobility: NA
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade diflufenican unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rats, >2000 mg/kg; mice, >1000 mg/kg, rabbits, >5000 mg/kg; Dermal LD_{50}, >2000 mg/kg; inhalation LC_{50}, > 2.34 mg/L air
Subchronic toxicity:
14-d NOEL rats = 1600 mg/kg/d; 90-d NOEL dogs >1000 mg/kg/d
Mutagenicity: Negative Ames test
Wildlife:
Bobwhite quail oral LD_{50}, >2150 mg/kg; Mallard duck oral LD_{50}, >4000 mg/kg; Daphnia 48-h LC_{50}, >10 mg/L; Rainbow trout 96-h LC_{50}, 56-100 mg/L; EC_{50} Daphnia magna, >10 mg/L (48 h); EC_{50} green algae 10 mg/L
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

diflufenzopyr

2-[1-[[[(3,5-difluorophenyl)amino]carbonyl]hydrazono]ethyl]-3-pyridinecarboxylic acid

CAS # Acid: 109293-97-2
Sodium salt: 109293-98-3

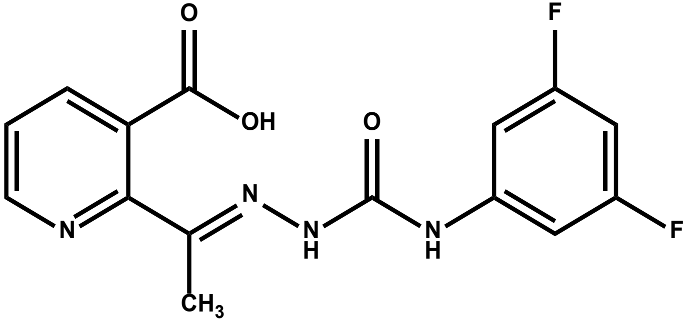
$19^{(P)}$

NOMENCLATURE

Common name: diflufenzopyr
Other name(s): 2-{(*EZ*)-1-[4-(3,5-difluorophenyl) semicarbazono]ethyl}nicotinic acid
Trade name(s): CELEBRITY® PLUS; DISTINCT®; OVERDRIVE®; STATUS®
Chemical family: semicarbazone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
diflufenzopyr



Molecular formula: *Acid* $C_{15}H_{12}F_2N_4O_3$; *Sodium salt* $C_{15}H_{11}F_2N_4NaO_3$
Molecular weight: *Acid* 334.28 g/mole; *Sodium salt* 356.26 g/mole
Description: Off-white powder
Density: 0.24 g/mL (25 C)
Melting point: 135.5 C
Boiling point: NA
Vapor pressure: 1.33×10^{-5} Pa (25 C); Henry's Law constant, 7.1×10^{-5} to 7.6×10^{-7} Pa m^3/mole
Stability: NA
Solubility: 270 mg/L (pH 5); 5850 mg/L (pH 7); 10,546 mg/L (pH 9)
pK_a: 3.18 (weak acid)
K_{ow}: 2.76 (pH 5); 0.34 (pH 7); 0.17 (pH 9)

HERBICIDAL USE

When diflufenzopyr is applied with dicamba, as in the DISTINCT Herbicide formulated product, it focuses dicamba's translocation to the meristematic sinks, where it delivers effective weed control at reduced dicamba rates and across a wider range of weed species. Sensitive broadleaf weeds exhibit rapid and severe plant hormonal effects (e.g., epinasty) after application of DISTINCT.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Diflufenzopyr is an auxin transport inhibitor. Diflufenzopyr inhibits the polar transport of naturally occurring auxin (indoleacetic acid, or IAA) and synthetic auxin-like compounds, such as dicamba, in sensitive plants. Diflufenzopyr's inhibition of auxin transport causes an abnormal accumulation of IAA and synthetic auxin agonists in meristematic shoot and root regions, disrupting the delicate auxin balance needed for plant growth. (more details on page 15)
Symptomology: Symptoms are visible within hours, and plant death usually occurs within a few days. Symptomology, in sensitive annual grasses, is characterized by a herbistatic stunting effect on growth. Tolerance in corn occurs through rapid metabolism of diflufenzopyr and dicamba.
Absorption/translocation: Absorbed by roots and leaves; translocated in phloem and xylem
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: None known
.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 18 to 156 mL/g
Transformation:
Photodegradation: Photolysis half-life: 14 d
Other degradation: DT_{50} 4 d
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade diflufenzopyr unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50}, 2.93 mg/L; Skin irritation rabbit, non-irritating; Eye irritation rabbit, minimal; Dermal sensitization guinea pig, not a sensitizer
Subchronic toxicity:
13-wk dietary, dog: NOEAL 58 mg/kg/d (1500 mg/kg)
Reproduction:
2-generation Wistar: NOAEL 100 mg/kg/d
Mutagenicity: Four acceptable mutagenicity studies were available for review: a microbial (*Salmonella typhimurium*) mutagenicity assay; an *in vitro* mammalian (mouse lymphoma) cell gene mutation assay; an *in vivo* mouse bone marrow micronucleus assay; and an unscheduled DNA synthesis assay. Diflufenzopyr was negative for mutagenic potential in all assays.
Wildlife:
Bobwhite quail oral LD_{50}, >2250 mg/kg; Mallard duck oral LD_{50}, >2250 mg/kg; Daphnia 48-h EC_{50}, non-toxic; Bluegill sunfish 96-h LC_{50}, non-toxic; Rainbow trout 96-h

LC

Aquatic – Freshwater: Diflufenzopyr is slightly toxic to practically non-toxic to freshwater organisms (LC_{50} = 15 to > 135 mg/L ae)

Aquatic - Estuarine/Marine: Diflufenzopyr is slightly toxic to practically non-toxic to estuarine/ marine organisms (LC_{50} or EC_{50} = 18.9 to > 138 mg/L ae)

Plants: Diflufenzopyr is highly toxic to terrestrial plants. Seedling emergence studies identified the turnip as the most sensitive dicot species (EC_{25} = 0.9 g acid equivalent/ha) and ryegrass as the most sensitive monocot (Shoot Length EC_{25} = 6.2 g ae/ha).

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF

Reference:

Lym, R.G. amd K.M. Christianson. 1998. Proc. West. Soc. Weed Sci. 51:59-62.

dimefuron

CAS #: 34205-21-5 $7^{(C_2)}$

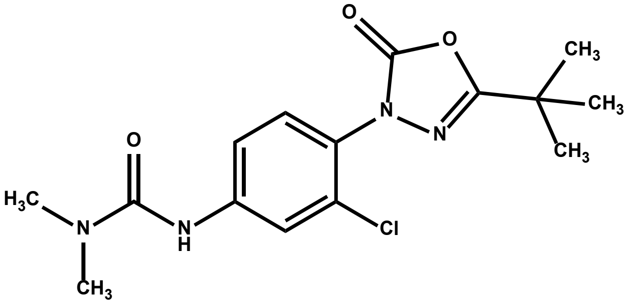
N′-[3-chloro-4-[5-(1,1-dimethylethyl)-2-oxo-1,3,4-oxadiazol-3(2H)-yl]phenyl]-N,N-dimethylurea

NOMENCLATURE

Common name: dimefuron
Other name(s): 23465 RP; 3-[4-(5-*tert*-butyl-2,3-dihydro-2-oxo-1,3,4-oxadiazol-3-yl)-3-chlorophenyl]-1,1-dimethylurea (IUPAC)
Trade name(s): PRADONE®
Chemical family: oxadiazolone; phenylurea; substituted urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:*dimefuron*



Molecular formula: $C_{15}H_{19}ClN_4O_3$
Molecular weight: 338.79 g/mole
Description: Colorless, odorless crystals
Density: NA
Melting point: 193 C
Boiling point: NA
Vapor pressure: 1×10^{-4} Pa (20 C)
Stability: Stable in aqueous solution
Solubility: In water, 16 mg/L (20 C); readily soluble in chloroform; moderately soluble in acetonitrile, acetophenone, ethanol; slightly soluble in benzene, toluene, xylene
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 2.51

HERBICIDAL USE

Applied PRE and POST at 0.2 to 2 kg ai/ha in field beans, certain cereals, cotton, peanut, dormant alfalfa, oilseed rape and peas.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis in photosystem II (PS II) (more details on page 13)
Symptomology: Chlorosis of affected foliage followed by necrosis and plant death.
Absorption/translocation: Absorbed by roots and leaves
Metabolism in plants: Demethylated dimefuron is the main metabolite.
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 117-262 mL/g
Transformation:
Other degradation: In aerobic soils, demethylated and hydroxylated *tert*-butyl metabolites of dimefuron are produced.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, > 2000 mg/kg; Dermal LD_{50} rabbit, 1000 mg/kg; non-sensitizer for skin or eye irritant
Subchronic toxicity:
90-d dietary, rat: NOEL 150 mg/kg/d
90-d dietary, dog: NOEL 20 mg/kg/d
Wildlife: NA
Use classification: WHO class V

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Feinchemie

dimethipin

CAS #: 55290-64-7

NC

2,3-dihydro-5,6-dimethyl-1,4-dithiin 1,1,4,4-tetraoxide

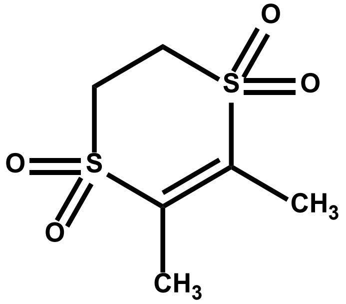
NOMENCLATURE

Common name: dimethipin (ISO)
Other name(s): N-252, SHA 118901; 2,3-dihydro-5,6-dimethyl-1,4-dithiine 1,1,4,4-tetraoxide (IUPAC)
Trade name(s): HARVADE 5F
Chemical family: None generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

dimethipin



Molecular formula: $C_6H_{10}O_4S_2$
Molecular weight: 210.26 g/mole
Description: colorless crystals with mild odor
Density: 1.59 g/mL
Melting point: 162-167 C
Boiling point: NA
Vapor pressure: 5.1×10^{-5} Pa (25 C)
Stability: Undergoes degradation in aqueous solution
Solubility: In water, 3 g/L (25 C). In acetone,180, xylene,10 (both g/kg at 25 C)
pK_a: 10.88 (weak base)
K_{ow}: 0.66

HERBICIDAL USE

Defoliation of cotton, nursery stock, rubber trees, and vines; used for post-directed control of morningglory and sicklepod in cotton.

USE PRECAUTIONS

Fire hazard: None known
Corrosiveness: Corrosive to metals
Storage stability: NA
Emergency exposure: Skin: wash affected area with soap and water
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Defoliant and desiccant
Symptomology: Foliar necrosis
Absorption/translocation: Non-systemic
Metabolism in plants: Not metabolized
Non-herbicidal biological properties: Rodenticide
Mechanism of resistance in weeds: No resistance reported

BEHAVIOR IN SOIL

Sorption:
K_d: 0.092 mL/g
K_{oc}: 3.27 mL/g
Persistence:
Field experiments: DT_{50} in soil 104-109 d
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dimethipin unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, 500 mg/kg; Dermal LD_{50} rabbit, > 5000 mg/kg; 4-h inhalation LC_{50} rates, 1.2 mg/L
Subchronic toxicity:
90-d dietary, rat: NOEL 2 mg/kg b.w. daily
90-d dietary, dog: NOEL 25 mg/kg b.w. daily
Wildlife:
Mallard duck and bobwhite quail LC_{50} (8 d), > 5000 mg/kg; rainbow trout LC_{50} (96 h), 52.8; bluegill sunfish, 20.9; sheepshead minnow, 17.8 mg/L; bees LD_{50}, >100 μg/bee; Daphnia LC_{50} (48 h), 21.3 mg/L; Earthworm LC_{50} (14 d), >39.4 mg/kg
Use classification: WHO Class III; EPA (formulation) I

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Uniroyal

dimethenamid

2-chloro-N-[(2,4-dimethyl-3-thienyl)-N-(2-methoxy-1-methylethyl)acetamide

CAS # unstated stereochemistry:
87674-68-8
S isomer: 163515-14-8

$15^{(K_3)}$

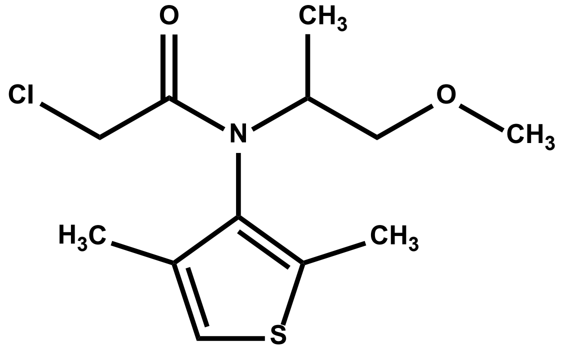
NOMENCLATURE

Common name: dimethenamid; dimethenamid-P (*S* isomer)
Other name(s): BAS 656H; SAN 582H; SAN 582; (*RS*)-2-chloro-*N*-(2,4-dimethyl-3-thienyl)-*N*-(2-methoxy-1-methylethyl)acetamide (IUPAC); (*S*)-2-chloro-*N*-(2,4-dimethyl-3-thienyl)-*N*-(2-methoxy-1-methylethyl)acetamide (dimethenamid-P, IUPAC); 2-chloro-*N*-(2,4-dimethyl-3-thienyl)-*N*-[(1*S*)-2-methoxy-1-methylethyl]acetamide
Trade name(s): FRONTIER®; GUARDSMAN®; GUARDSMAN MAX®; GMAX-LITE™; OPTILL®; OUTLOOK®; LEADOFF®
Chemical family: acetamide; acetanilide; amide; chloroacetamide; chloroacetanilide

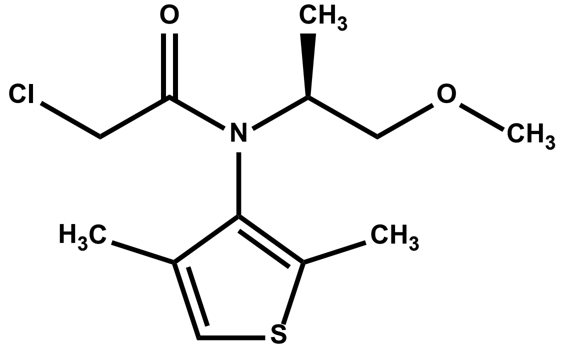
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

dimethenamid



dimethenamid-P



Molecular formula: $C_{12}H_{18}ClNO_2S$
Molecular weight: 275.79 g/mole
Description: Dark brown viscous liquid, weak “tar-like” odor
Density: 1.19 g/mL (25 C)
Melting point: NA
Boiling point: >250 C (1.01 x 10^5 Pa); 123 C (13.3 Pa)
Vapor pressure: 3.68 x 10^{-2} Pa (25 C)
Stability: Stable for 90 d (55 C)
Solubility:
water 1174 mg/L (25 C)
organic solvents g/100 mL (25 C):
heptane 26.7
isooctane 19.4
Completely miscible in:
acetone
carbon disulfide
DMSO
n-hexane
methylene chloride
2-propanol
Toluene
acetonitrile
dimethylformamide
ethyl acetate
methanol
n-octanol
tetrahydrofuran
p-xylene
pK_a: None (non-ionizable)
K_{ow}: 141 ± 6 (25 C)

HERBICIDAL USE

Dimethenamid can be applied early preplant, PPI, PRE, or early POST at 0.85-1.64 kg ai/ha in corn and soybeans to control many annual grasses such as foxtail spp., barnyardgrass, fall panicum, and crabgrass spp., as well as yellow nutsedge and certain annual broadleaf weeds including redroot pigweed and black nightshade. Dimethenamid can be applied by conventional sprayer in water or liquid fertilizer, or can be impregnated on dry bulk fertilizer. Early POST applications have little to no activity on emerged weeds. Dimethenamid can also be use PPI, PRE, and early POST in dry beans, peanuts and PRE or POST in established grass grown for seed, and PPI or PRE in grain sorghum.

USE PRECAUTIONS

Fire hazard: Technical, FRONTIER, and GUARDSMAN are non-flammable; flash points are 91°C, 78 C and >102 C (Pensky-Martens closed cup), respectively.
Corrosiveness: Technical, FRONTIER, and GUARDSMAN corrode C1020 steel at 0.058, 0.069, and 0.043 mm/yr, respectively, at 55 C
Storage stability: Technical was stable for 2 yr in glass at 25 C and for 3 yr in an HDPE drum at warehouse temperature. FRONTIER and GUARDSMAN were stable after 2 yr at 25°C.
Cleaning glassware/spray equipment: Wash equipment with detergent and rinse. Acetone can be used for glassware.
Emergency exposure: Flush eyes with water for 15 min and wash skin with soap and water; get medical attention if irritation persists. If FRONTIER is ingested, drink 1-2 glasses of water and induce vomiting; seek medical attention. Treat symptomatically.
Incompatibilities: Avoid contact with strong oxidizers. A compatibility agent may be required when mixing FRONTIER with triazine herbicides plus liquid fertilizer.

BEHAVIOR IN PLANTS

Mechanism of action: Thought to be inhibition of very long chain fatty acid synthesis (VLCFA) (1) (more details on page 14)

Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Injury on corn and sorghum can be caused by excessive dimethenamid rates and appears as malformed and twisted seedlings. Leaves are tightly rolled in the whorl and may not unroll normally. Injured soybean seedlings may have cupped or crinkled leaves. New leaves may have a shortened midrib producing a "drawstring" or "heartshape" appearance.

Absorption/translocation: Absorbed primarily by emerging grass shoots (coleoptile) and by emerging broadleaf shoots and roots. Translocation is established plants is irrelevant to mechanism of action because dimethenamid is phytotoxic only to emerging seedlings.

Metabolism in plants: Rapidly and extensively metabolized in corn and soybeans to about 30 metabolites. Residues in corn and soybean raw agricultural commodities consist of numerous highly polar metabolites, each at <0.01 mg/kg (LOD) in the samples and not representing more than 10% of the applied dimethenamid.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to soil

K_{oc} K_f, and 1/n: K_{oc}, K_f and 1/n were 55 mL/g, 2.4 mL/g and 0.9, respectively, for adsorption and 165 mL/g, 2.6 mL/g, and 0.89, respectively, for desorption of non-aged residues on four soils with pH 6.4-7.4, OM content of 0.5-4.9%, and 12-36% clay K_{oc}, K_f, and 1/n were 125 mL/g, 0.8 mL/g, and 1.11, respectively, for adsorption and 1468 mL/g, 6.7 mL/g, and 1.21, respectively, for desorption of residues aged for 30 d on four soils with pH 6.5-7.5, OM content of 0.5-2.6%, and 4-28% clay

Transformation:

Photodegradation: Rate constant was 0.089/d and half-life was 8 d on dry soil at 25 C exposed to continuous simulated high intensity sunlight in the lab. Photodegradation has little impact on overall field dissipation.

Other degradation: Primarily degraded by microbes. In the lab, dimethenamid degraded in sterile and non-sterile soils with half-lives of 377 and 38 d, respectively, at 25 C. Oxalamide was the major degradation product (in lab as well as field studies). Half-life increased under anaerobic conditions or when temperature was lowered to 5 C. Dimethenamid was not hydrolyzed in water buffered at pHs 5, 7, and 9, and at 25 C for 30 d. Non-microbial hydrolysis appears to be an insignificant contributor to field dissipation.

Persistence: Half-life averaged 20 d over 10 field studies in North America and Europe, but ranged from 1-2 wk in the southern U.S. to 5-6 wk in the northern U.S. Residues from spring-applied dimethenamid do not injure fall-seeded cereal crops and do not injure other crops planted the following season.

Mobility: Neither dimethenamid nor its degradation products have been found below 10 cm in soil. These results, together with the GUS factor and PRZM worst-case simulation, suggest that dimethenamid does not pose an unacceptable risk to groundwater.

Volatilization: Low losses; soil incorporation is not required

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dimethenamid unless otherwise indicated

Acute toxicity:

Oral LD_{50} rat, 1570 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >4.99 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, slight; Eye irritation rabbit, slight

FRONTIER: Oral LD_{50} rat, 2400 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >3.9 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, slight-severe

GUARDSMAN: Oral LD_{50} rat, 1293 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 2 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, mild

Subchronic toxicity: NA

90-d dietary, rat: NOEL 7.5 mg/kg/d

90-d dietary, dog: NOEL 2.5 mg/kg/d

21-d dermal, rabbit: NOEL 500 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 4.5 mg/kg/d; not carcinogenic at up to 3000 mg/kg; liver effects

24-mo dietary, rat: NOEL 5 mg/kg/d; statistically no significant trend for increased incidence of liver tumors in male at 1500 mg/kg; liver effects

12-mo dietary, dog: NOEL 6.25 mg/kg/d

Teratogenicity:

Rat: NOEL maternal 50 mg/kg/d, developmental 215 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 37.5 mg/kg/d, developmental 75 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL parental 10 mg/kg/d, pups 25 mg/kg/d in a 2-generation study

Mutagenicity:

Gene mutation: Ames, test, negative

Structural chromosome aberration: CHO, negative but suggestive of a positive clastogenic response; Mouse bone marrow/micronucleus, negative

DNA damage/repair: Rat primary hepatocytes/UDS, positive in one assay but this was not confirmed in two additional assays

Mammalian cell transformation: BALB/3T3 cells, negative

Wildlife:

Bobwhite quail LD_{50}, 1908 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Earthworm 14-d LC_{50} in soil, 294.4 mg/kg; Honey bee, oral LD_{50}, >1000 μg/bee, topical LD_{50}, 94 μg/bee; Daphnia 48-h LC_{50}, 16 mg/L; Daphnia life cycle LOEC, 2.51 mg/L, NOEC, 1.36 mg/L, MATC, 1.85 mg/L; Bluegill sunfish 96-h LC_{50}, 6.4 mg/L; Minnow 96-h LC_{50}, 7.2 mg/L; Rainbow trout 96-h LC_{50}, 2.6 mg/L, early life stage NOEC, 0.12 mg/L, LOEL, 0.24 mg/L, MATC, 0.17 mg/L; Oyster

96-h EC_{50}, 5 mg/L; Shrimp 96-h LC_{50}, 4.8 mg/L; *Lemna gibba* 72-h EC_{50}, 0.051 mg/L; *Selanstrum capricormutum* 72-h EC_{50}, 0.122 mg/L; *Anabaena flosaguae* 72-h EC_{50}, 0.35 mg/L; *Navicula pelliculosa* 72-H EC_{50}, 1.2 mg/L; *Skeletonema costalum* 72-h EC_{50}, 0.04 mg/L

FRONTIER: Rainbow trout 96-h LC_{50}, 2.1 mg/L

Use classification: General use for Frontier. Restricted use for GUARDSMAN due to groundwater contamination concerns with atrazine

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Dimethenamid from soil or grain (corn and soybeans) samples with 5% methanol, followed by solid phase extraction in a C_{18} cartridge. The eluted solution is further cleaned-up using diatomaceous earth and silica gel columns, and then concentrated for analysis. Dimethenamid can be analyzed separately or together with its oxalamide metabolite in soil, corn, or soybeans using GC with either nitrogen phosphorous detection or mass selective detection. The oxalamide metabolite is analyzed separately (or together with parent dimethenamid) after conversion to its methyl ester with methanol sulfuric acid or diazomethane. Clean-up steps are similar to those used for parent dimethenamid with the addition of a cation exchange cleanup. The sulfonate metabolite is extracted in 2% methanol, and the extracts cleaned-up with cation exchange solid phase extraction. The extracts are then eluted through an anion exchange column, concentrated, and analyzed by HPLC with a C_{18} column.

Historical: Dimethenamid was synthesized, discovered, patented (U.S. patent 4,666,502), and developed by Sandoz Agro Ltd. FRONTIER was registered for use in corn in March 1993 and was registered in soybeans in March 1994 (Canada registration in both crops was received in January 1994). GUARDSMAN received registration in corn in November 1993.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): BASF

Reference(s):

1. Böger, P., B. Matthes, and J. Schmalfuss. 2000. Pest. Manag. Sci. 56:497-508.

dinoterb

2-(1,1-dimethylethyl)-4,6-dinitrophenol

CAS #: 1420-07-1
Acetate: 32004-27-1

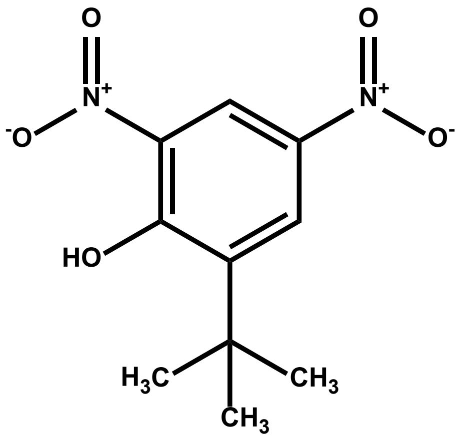
$24^{(M)}$

NOMENCLATURE

Common name: dinoterb (ISO)
Other name(s): LS63133; P 1108; 2-tert-butyl-4,6-dinitrophenol
Trade name(s): HERBOGIL
Chemical family: dinitrophenol

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
dinoterb



Molecular formula: $C_{10}H_{12}N_2O_5$; *acetate* $C_{12}H_{14}N_2O_6$
Molecular weight: 240.22 g/mole
Description: Pale yellow solid with a phenol-like odor
Density: NA
Melting point: 125.5-126.5 C
Boiling point: NA
Vapor pressure: 2×10^{-2} Pa (20 C)
Stability: Stable below the melting point; de-composes above (220 C); stable at least 34 d at pH 5-9 (22 C)
Solubility: In water 4.5 mg/L (pH 5, 20 C); in cyclohexanone, ethyl acetate, dimethyl sulfoxide approximately 200 g/kg; in alcohols, glycols, aliphatic hydrocarbons approximately 100 g/kg; soluble in aqueous alkalis with the formation of salts.
pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

Dinoterb is used for control of annual broad-leaved weeds postemergence in cereals, maize, alfalfa, and beet; and preemergence in peas and beans. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Oxidative phosphorylation uncoupler (more details on page 15)
Symptomology: Contact-type necrosis on foliage
Absorption/translocation: Non-systemic, contact-type herbicide
Metabolism in plants: NA
Mechanism of resistance in weeds: No resistance reported.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
  Photodegradation: NA
  Other degradation: NA
Persistence: NA
Mobility: NA
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dinoterb unless otherwise indicated.

Acute toxicity:
  Oral LD_{50} rat, 62 mg/kg; Dermal LD_{50} guinea pig, 150 mg/kg
Chronic toxicity:
  24-mo dietary, rats: NOEL 0.375 mg/kg diet.
Wildlife:
  Rainbow trout LC_{50} (96 h) 0.0034 mg/L; toxic to bees
Use classification: WHO class I

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA
Analytical methods: Gas chromatography (1)
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1. Dekker, W.H. and H.A. Selling. 1975. J. Agric. Food Chem. 23: 1013.

diquat

6,7-dihydrodipyrido[1,2-*a*:2′,1′-*c*]pyrazinediium

CAS# Cation: 2764-72-9
Dibromide salt: 85-00-7

$22^{(D)}$

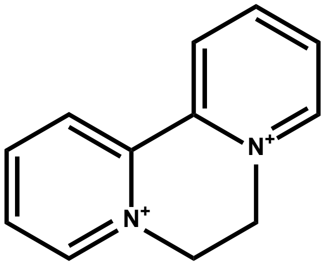
NOMENCLATURE

Common name: diquat (ANSI, BSI, ISO, WSSA)
Other name(s): deiquat; FB/2; 1,1′-ethylene-2,2′-bipyridyldiylium (IUPAC);
Trade name(s): REGLONE®; AQUACIDE; DEXTRONE; REWARD; WEEDTRINE®; QUICKPRO®
Chemical family: bipyridilium; bipyridinium; dipyridilium; quaternary ammonium

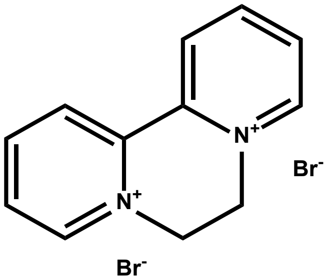
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure

diquat cation



Diquat dibromide salt



Molecular formula: *Cation* $C_{12}H_{12}N_2$; *Dibromide salt* $C_{12}H_{12}Br_2N_2$
Molecular weight: *Cation* 184.24 g/mole; *Dibromide salt* 344.05 g/mole
Description: Yellow crystalline solid (pure salt monohydrate)
Density: 1.61 g/mL (25 C)
Melting point: 325 C
Boiling point: NA
Vapor pressure: $<1.3 \times 10^{-5}$ Pa (25 C)
Stability: Degraded by UV light; decomposes above 300 C; decomposes in alkaline solution, but is stable in neutral or acidic solution
Solubility:

water 718,000 mg/L (pH 7.2, 20 C)
organic solvents g/100 mL (20 C):
acetone <0.01
ethanol slightly soluble

benzene insoluble	*n*-hexane 0.01
chloroform insoluble	methanol slightly soluble
diethyl ether insoluble	toluene <0.01

pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = -4.26(20 C)

HERBICIDAL USE

Diquat can be applied POST spray-to-wet using 240 g cation/100 L water to control cattails. Diquat also can be applied to ponds, lakes, and drainage ditches for control of algae, submersed aquatic weeds such as bladderwort, coontail, and *Elodea*, and floating aquatic weeds such as pennywort, salvinia, and water hyacinth.

USE PRECAUTIONS

Fire hazard: The product DIQUAT is aqueous and nonflammable.
Corrosiveness: Dilute spray solutions of DIQUAT are noncorrosive to all materials commonly used in spray equipment; concentrated solutions corrode aluminum rapidly. Undiluted diquat should not be stored in contact with metals.
Storage stability: Stable at 54 C for 14 d. Shelf life is indefinite under normal storage conditions. Diquat technical is somewhat sensitive to UV light. The product is stable to heat beyond ordinary ambient temperatures. The solution does not crystallize at 0 C.
Cleaning glassware/spray equipment: Flush equipment with water
Emergency exposure: If ingested, induce vomiting and get medical attention immediately. Perform gastric lavage and give repeated suspensions of activated charcoal together with saline purgatives. Removal of diquat from the blood requires prolonged charcoal hemoperfusion.
Incompatibilities: Incompatible with some alkyl sulfonate or alkyl aryl sulfonate wetting agents or alkali metal salts of hormone weed killers. Diquat may hydrolyze in the presence of alkaline materials including alkaline water. DIQUAT may be mixed with 2,4-D, substituted ureas, uracils, dalapon, and *s*-triazines.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem I (PS I) (more details on page 15)
Symptomology: Rapid wilting and desiccation beginning within several h of application in full sunlight. Complete foliar necrosis occurs in 1-3 d.
Absorption/translocation: Rapidly absorbed into leaves and is rainfast within 1 to 2 h. More than 50% of applied diquat was absorbed by leaves of three species within 1 h (1). Diquat translocates in the apoplast, but rapid cell death following absorption along with the normal upward movement of xylem flow usually prevents appreciable translocation from treated leaves. Under certain conditions favoring downward xylem movement, diquat may translocate out of treated leaves and into roots of potatoes.
Diquat is tightly adsorbed to negatively charged leaf surfaces and membranes due to its positive charge and highly polar nature.

Metabolism in plants: Diquat apparently is not metabolized in higher plants, although it can be photodegraded on plant surfaces (4).

Non-herbicidal biological properties: No fungicide, nematocide, or insecticide activity. Diquat is highly toxic to mammals.

Mechanism of resistance in weeds: Most paraquat-resistant biotypes are resistant to diquat, although often at substantially reduced levels. High levels of diquat resistance have occurred in biotypes of capeweed (*Arctotheca calendula*) and horseweed. Resistance mechanisms have not been determined, but may be similar to the protective or sequestration mechanisms proposed for paraquat resistance (3).

BEHAVIOR IN SOIL

Sorption: Extremely tightly adsorbed to (negatively-charged) soil particles due to its dicationic nature. Diquat is primarily adsorbed to clay, less so to OM. Diquat bound to soil is unavailable for plant uptake and is largely unavailable to soil microbes.

K_{oc}: Average is 1,000,000 mL/g (estimated) (5)

Transformation:

Photodegradation: Losses probably occur on sprayed leaf surfaces and on dead and decaying vegetation. Photochemical decomposition of diquat has been measured in the lab by irradiating thin layers of soil, but has not been unequivocally demonstrated under field conditions.

Other degradation: Certain microbe species in soil-less culture media decompose diquat. However, they degrade diquat bound to soil slowly or not at all.

Persistence: Typical half-life is 1000 d (5). Diquat is highly persistent due to strong binding to clay and unavailability to microbes. Diquat in soil is not taken up by plants, so any crop can be seeded at any time after application.

Mobility: Immobile in soil

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade diquat dibromide salt unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 230 mg/kg; mouse, 125 mg/kg; dog, 100-200 mg/kg; cow, 30 mg/kg; Dermal LD_{50} rabbit, >400 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

Subchronic toxicity: NA

Chronic toxicity:

18-mo dietary, mouse: NOEL NA; not carcinogenic after ~100 wk at 36 mg/kg; not oncogenic at 36 mg/kg/d; not carcinogenic

12-mo dietary, dog: NOEL 50 mg/kg; cataracts after 15 mo at 150 mg/kg; not carcinogenic

Teratogenicity: NA

Reproduction:

Rat: NOEL NA; not a reproductive toxin; growth retardation at 25 mg/kg/d

Mutagenicity: NA

Wildlife:

Hen oral LD_{50}, 200-400 mg/kg; Partridge oral LD_{50}, 295 mg/kg; Mirror carp 96-h LC_{50}, 67 mg/L; Rainbow trout 96-h LC_{50}, 21 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 2,2′-bipyridyl is reacted with di-*n*-propyl amine.

Purification of technical: Recrystallization from water or aqueous solvent mixtures. Diquat dibromide monohydrate may be isolated from the formulated product as follows: Slightly acidify with hydrobromic acid. Add 10 volumes of acetone to each volume of the diquat formulation and stir vigorously. Filter and rinse the yellow solid diquat dibromide monohydrate with acetone. Further purify by dissolving the precipitate in a minimum of water, acidifying with hydrobromic acid, and repeating the precipitation with 10 volumes of acetone.

Analytical methods: Methods for formulated product and residue analysis are available (6), and are based on spectrophotometric measurement.

Historical: First made by Dyestuffs Division of I.C.I., Ltd. First used in 1955 as a growth regulator. British patent 785,732 was applied for in 1955.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Applied Biochemists; Syngenta Crop Protection

Reference(s):

1. Brian, R. C. 1967. Ann. Appl. Biol. 59:91.
2. Dodge, A. D. 1982. Pages 57-77 *in* D. E. Moreland, J. B. St. John, and F. D. Hess, eds., Biochemical Responses Induced by Herbicides. Am. Chem. Soc. Symp. Ser. No. 181, Washington, D.C.
3. Dodge, A. D. 1991. Pages 165-176 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Oxford.
4. Funderburk and Lawrence. 1964. Weeds 12:259.
5. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
6. Zweig, G., ed. 1967. Analytical Methods for Pesticides, Plant Growth Regulators and Food Additives, Vol. 5. Academic Press, New York.

dithiopyr

CAS #: 97886-45-8 3$^{(K_1)}$

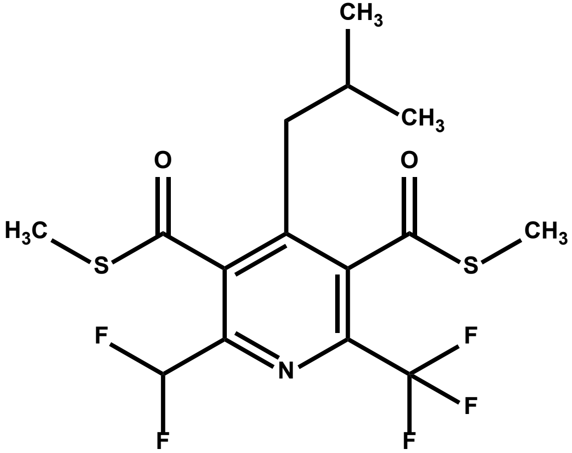
S,*S’*-dimethyl 2-(difluoromethyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-3,5-pyridinedicarbothioate

NOMENCLATURE

Common name: dithiopyr (ANSI, ISO,WSSA)
Other name(s): MON 7200; MON 15100; MON 15151; RH-101664; 3,5-pyridinedicarbothioic acid, 2-(difluoromethyl)-4-(2-methypropyl)-6-(trifluoromethyl)-S,S-dimethylester; S,S’-dimethyl-2-difluoromethyl-4-isobutyl-6-trifluoromethylpyridine-3,5-dicarbothioate (IUPAC)
Trade name(s): DIMENSION®; DITHIOPYR®, PRO-MATE®; STAKEOUT
Chemical family: amide; pyridine; substituted amide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
dithiopyr



Molecular formula: $C_{15}H_{16}F_5NO_2S_2$
Molecular weight: 401.41 g/mole
Description: Crystalline colorless, faint odor
Density: 1.42 g/mL (20 C)
Melting point: 65 C
Boiling point: 52 C (1.01 x 10^{-5} Pa)
Vapor pressure: 5.33 x 10^{-4} Pa (25 C)
Stability: >2 yr (>0 C)
Solubility:
water 1.38 mg/L (20 C)
pK_a: None (non-ionizable)
K_{ow}: 56,250

HERBICIDAL USE

Dithiopyr is applied PRE at 0.056-0.56 kg ai/ha or POST at 0.14-0.56 kg ai/ha in direct-seeded and transplanted rice; PRE at 0.14-0.56 kg ai/A or POST at 0.56 kg ai/ha in established turf [maximum single application to turf is 0.56 kg ai/ha] with total amount not to exceed 1.68 kg ai/ha and PRE at 0.14-2.24 kg ai/ha in ornamentals, trees, and other perennial crops. Dithiopyr controls several annual grass and small-seeded broadleaf weeds such as barnyardgrass, crabgrass spp., goosegrass, Oxalis, and spurge.

USE PRECAUTIONS

Fire hazard: Technical and DIMENSION EC are non-flammable; flash points are 84 C and 63 C, respectively.
Corrosiveness: Copper, iron, and zinc were not corroded after a 2-wk exposure to DIMENSION EC in sunlight at 52 C.
Storage stability: Technical and dithiopyr granules are stable. DIMENSION EC may crystallize below 0 C but can be re-dissolved by shaking at temperatures >15 C.
Cleaning glassware/spray equipment: NA
Emergency exposure: If ingested, do not induce vomiting. Drink large quantities of water and get medical attention. Dimension EC is severely irritating to eyes and skin.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits mitosis in late prometaphase. Dithiopyr does not bind to tubulin but to another protein that may be a microtubule associated protein (MAP). MAPs function in microtubule stability. Dithiopyr results in shortened microtubules that cannot form the spindle fibers normally responsible for separating chromosomes to the poles of the cell during mitosis. Cortical microtubules, which normally prevent isodiametric cell expansion, also are essentially absent resulting in club-shaped root tips (1). (more details on page 12)
Symptomology: Dithiopyr causes swelling in meristematic regions such as root tips.
Absorption/translocation: Absorbed by roots and to some degree by the foliage of susceptible plants. The most important site of uptake appears to be meristematic regions since dithiopyr translocation is limited and the primary site of action seems to be meristematic tissues.
Metabolism in plants: Rice treated 1 day after transplanting at 1.4 kg/ha resulted in non-detectable residues in grain. The major component in forage and straw was unchanged dithiopyr (29% of the TRR (0.006 mg/kg), and 9% of the TRR (0.002 mg/kg), respectively). Dithiopyr is metabolized first to the two monoacids, then to the diacid, same as in soils.
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil. Sorption is somewhat reversible on low OM soils.

K_{oc}: Average is 1638 mL/g
K_d: 7.89 mL/g for a Sappy sandy loam soil with 0.58% OC, 0.8% OM 8% clay, and pH 8; 12.82 mL/g for a Dupo silt loam soil with 0.74% OC, 1% OM, 8% clay, and pH 7.5; 45.93 mL/g for a Sharkey clay soil with 1.85% OC, 3.2% OM, 59% clay, and pH 6.2
K_f and 1/n: K_f 6.59 mL/g and 1/n 0.93 for a Sappy soil; Kf 7.91 mL/g and 1/n 0.83 for a Dupo soil; Kf 26.92 and 1/n

0.86 for a Sharkey soil

Transformation:

Photodegradation: Only 5% of dithiopyr was photolyzed to a monoacid after application at 1.12 kg ai/ha to soil and an exposure in Pyrex equivalent to 33.6 d of sunlight at 25 C from a xenon arc lamp producing 198 mW/m^2 from 300-750 nm. Half-life was 17.6 d for dithiopyr at 0.7 ppm in buffered water without photosensitizers in Pyrex at 25 C, and primary metabolites were the two monoacids and the diacid.

Hydrolysis: stable at pH 5, 7 and 25 C for 30 days; at pH 9 <2% monoacid II was produced

Other degradation: Dithiopyr is microbially degraded slowly in soil to the two monoacids and the diacid (each at <6% of applied radioactivity at 12 months), respectively as follows: 3-pyridinecarboxylic acid, 2-(difluoromethyl)-4-(2-methylpropyl)-5-[(methyl-thio)carbonyl]-6-(trifluoromethyl)-(monoacid II); 3-pyridine carboxylic acid, 6-(difluoromethyl)-4-(2-methylpropyl)-5-[(methyl-thio) carbonyl]-2-(trifluoromethyl)- (monoacid III); and 3,5 pyridine dicarboxylic acid, 2-(difluoromethyl)-4-(2-methylpropyl)-6(trifluoromethyl)- (diacid IV). Bound resides are minimal with 4% of applied dithiopyr remaining in the soil after Soxhlet extraction.

Persistence: Somewhat short to moderate field persistence.

Field experiments: Half-life was 17 d when applied as an EC, with a range of 3-49 d across 14 turf sites representing diverse climes, soil textures, and irrigation methods. Metabolites were dissipated almost completely within 1 yr.

Mobility: Leaching of dithiopyr and its acid metabolites did not exceed 61 cm, and was often <23-30 cm even in sandy soil with low OM content and 249 cm of irrigation. Dithiopyr and its metabolites were not detected at >10 mg/L between 61 and 244 cm. Groundwater Ubiquity Score (GUS) for dithiopyr is <1.8 and is therefore classified as a non-leacher. This is corroborated by a 5 year ground water monitoring study of 40 wells located on vulnerable sandy soils on Long Island, NY, which resulted in no detections of dithiopyr or its metabolites above the method LOQ (1 ug/L). Potential for movement in runoff water is unlikely due to low water solubility and strong adsorption to turfgrass and soil.

Volatilization: In a field study, volatilization rate declined from 2% h immediately after application to 0.1% h 3 d after application. Total losses were 6.2-18.7% of applied during the first 3 d after application and were 12-40% during the 30-d study. Dithiopyr oxidizes rapidly in the atmosphere (DT50<2 days) via reaction with hydroxyl radicals.

Formulation effects: Half-life of emulsifiable concentrate, microencapsulated and granule formulation averaged 17, 36, and 61 d, respectively. These different half-lives presumably reflect differing volatilization losses.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade dithiopyr unless otherwise indicated.

Acute toxicity:

Oral LD50 rat, >5000 mg/kg (EPA Cat. IV); Dermal LD50 rabbit >5000 mg/kg (EPA Cat. IV); 4-h inhalation LC50 rat, >6 mg/L (EPA Cat. IV); Skin irritation rabbit, slight, resolved by 72 hours (EPA Cat. IV); Skin sensitization guinea pig, non- sensitizer; Eye irritation rabbit, slight, resolved within 24 hours (EPA Cat. IV)

DIMENSION: Oral LD50 rat, 3600 mg/kg (EPA Cat. III); Dermal LD50 rabbit, >5000 mg/kg (EPA Cat. IV); 4-h inhalation LC50 rat, 11 mg/L (EPA Cat. IV); Skin irritation rabbit, severe (EPA Cat II); Skin sensitization guinea pig, non-sensitizer; Eye irritation rabbit, severe (EPA Cat. II)

DIMENSION 0.25G: Oral LD50 rat, >5000 mg/kg (EPA Cat. IV); Dermal LD50 rabbit, >5000 mg/kg (EPA Cat. IV); Skin irritation rabbit, none (EPA Cat. IV); Skin sensitization guinea pig, non-sensitizer; Eye irritation rabbit, slight (EPA Cat. IV).

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: Lung cells, negative

DNA damage/repair: Primary hepatocytes, negative

In vivo chromosome aberration: micronucleus, negative

Subchronic toxicity:

90-day dietary, rat: NOEL 10 ppm in females and 100 ppm in males; Effects on liver and kidney at ≥ 100 ppm

90-day dietary, dog: NOEL 1 mg/kg/day; liver toxicity at ≥ 10 mg/kg/day

Chronic toxicity:

18-month dietary, mouse: NOEL 3 ppm; liver and adrenal gland weight increases at ≥ 30 ppm; increased splenic hematopoiesis, adrenal changes, and evidence of cholestasis at 300 ppm; not carcinogenic

24-month dietary, rat: NOEL 10 ppm; liver and kidney weight increases at 300 ppm; not carcinogenic

12-month dietary, dog: NOEL 0.5 mg/kg/day; slight liver toxicity at 5 mg/kg/day

Teratogenicity:

Rat and rabbit: Developmental NOEL 1000 mg/kg/day; toxicity in dams at 1000 mg/kg/day; non-teratogenic

Reproduction:

Rat: Parental NOEL 25 ppm; decreased weight gain, liver and kidney weight increases, and histopathological evidence of liver; kidney, thyroid, and adrenal toxicity at 250 and 2500 ppm; no effects on reproductive performance effects on reproductive performance

Wildlife:

Bobwhite quail oral LD$_{50}$ >2250 mg/kg; 5-d dietary LC$_{50}$ >5620 mg/kg; reproductive NOEC ≥1250 mg/kg; mallard duck 5-d dietary LC$_{50}$ >5620 mg/kg; reproductive NOEC 250 mg/kg; earthworm LC$_{50}$ in soil >1000 mg/kg; honeybee topical 48-h LC$_{50}$ 81 µg/bee; algae 5-d EC$_{50}$ 52.9 µg/L; Daphnia 48-h LC$_{50}$ >1.7 mg/L; 21-d NOEC 0.081 mg/L; mysid shrimp 96-h LC$_{50}$ 0.586 mg/L; bluegill sunfish 96-h LC$_{50}$ 0.7 mg/L; carp 96-h LC$_{50}$ 0.72 mg/L; sheepshead minnow 96-h LC$_{50}$ 2.2 mg/L; rainbow trout 96-h LC$_{50}$ 0.48 mg/L; early life stage (ELS) 60-d NOEC 0.056 mg/L; fathead minnow full lifecycle test 272-d NOEC ≥ 0.039 mg/L.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods:

Dithiopyr and Metabolite Analysis in Soil: The parent compound, dithiopyr, is selectively extracted from soil by first shaking the sample with a 95% solution of acetonitrile/0.2 M HCl and secondly with petroleum ether (PE). The PE phase containing dithiopyr is retained for further cleanup. The aqueous phase containing all the acidic metabolites is acidified, and then partitioned into diethyl ether (DE), followed by methylation with diazomethane. Water is added to the methylated solution, and methylated metabolites are extracted from the aqueous solution with PE. The extracts of the parent compound dithiopyr and the methylated metabolites are then combined and purified using a Florisil column. This combined extract is brought to final volume in isooctane. Quantitation is performed by gas liquid chromatography using electron capture detection (GLC/ECD).

Dithiopyr and Metabolite Analysis in Water: The parent residue is separated from the metabolites in a base liquid-liquid partition. The metabolites are then extracted from the water sample using an acid liquid-liquid partition. The metabolites can then be methylated using diazomethane. The methylated samples are then recombined with the parent samples and are further purified by Florisil column chromatography. Quantitation of all compounds is performed by gas-liquid chromatography using electron capture detection (GCIECD) on an Rtx-200 column and confirmed by gas-liquid chromatography using electron capture detection on an Rtx-2330 column.

Historical: First introduced by Monsanto Company, but purchased by Rohm and Haas in 1994. Dithiopyr is covered by U.S. patent 4,692,184.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Dow AgroSciences; Helena; Monsanto **Reference(s):**

1. Vaughn and Lehnen. 1991. Weed Sci. 39:450.

diuron

N′-(3,4-dichlorophenyl)-N,N-dimethylurea

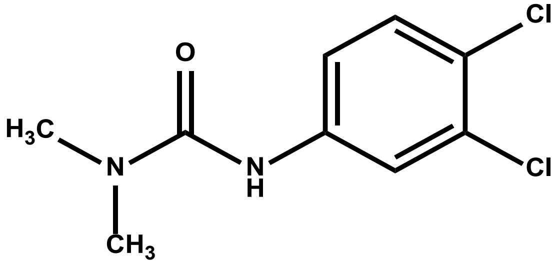
CAS #: 330-54-1 **$7^{(C_2)}$**

NOMENCLATURE

Common name: diuron (ANSI, BSI, ISO, WSSA)
Other name(s): dichlorfenidim; 3-(3,4-dichlorophenyl)-1,1-dimethylurea (IUPAC)
Trade name(s): ADIOS™ , CUTOUT®; BAREGROUND BD; CORSAGE®; DETERMINE®;DIREX® 4L; DIREX® 80 DF; DIURON 4L; GINSTAR® EC; HERBON PINK; KARMEX® DF; KARMEX® IWC; KARMEX® XP; KROVAR® I DF; PARROT®
Chemical family: phenylurea; substituted urea; urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
diuron



Molecular formula: $C_9H_{10}Cl_2N_2O$
Molecular weight: 233.10 g/mole
Description: White, crystalline solid, odorless
Density: NA
Melting point: 158-159 C
Boiling point: NA
Vapor pressure: 9.2×10^{-6} Pa (25 C); 4.1×10^{-4} Pa (50 C); 1.9×10^{-1} Pa (100 C)
Stability: Decomposes (180-190 C)
Solubility:
water 42 mg/L (25 C)
organic solvents g/100 mL (27 C):

acetone 4.2	butyl stearate 0.14
benzene 0.105	refined cottonseed oil 0.09

pK_a: None (non-ionizable)
K_{ow}: 589

HERBICIDAL USE

Diuron can be applied as follows: PRE at 0.9-3.6 kg ai/A in established alfalfa and established asparagus; PRE at 1.8 kg ai/ha in established birdsfoot trefoil; PRE at 0.6-0.9 kg ai/ha in corn (AR, LA, MS, TN only); POST-directed at 1.8-3.6 kg ai/ha in artichokes; POST-directed at 0.67-0.9 kg ai/ha in field corn; POST-directed at 0.22-0.45 kg ai/ha in grain sorghum; PRE at 1.8-7.2 kg ai/ha or POST-directed at 0.45-1.8 kg ai/ha in sugarcane; PRE at 1.3-1.8 kg ai/ha in winter barley (OR and WA only); PRE at 0.9-2.7 kg ai/ha in newly-sprigged bermudagrass pastures; preplant at 0.6-2.2 kg ai/ha in irrigated cotton (AZ, CA only); PRE at 0.6-2.2 kg ai/ha in dryland cotton; PRE at 1.8-3.6 kg ai/ha in pears and established perennial grass seed crops; PRE or POST at 0.9-1.3 kg ai/ha in spring oats; PRE at 1.3-1.8 kg ai/ha in winter oats; PRE at 2.7 kg ai/ha in established peppermint and plumosus fern; PRE at 1.8 kg ai/ha in olives (CA only) and established red clover; PRE or POST at 1.3-1.8 kg ai/ha in winter wheat; PRE at 1.8-2.7 kg ai/ha in apples; PRE at 1.3-2.7 kg ai/ha in bananas and plantains; PRE at 1.3-3.6 kg ai/ha in pecans, blueberries, caneberries, and gooseberries; PRE at 1.8-7.2 kg ai/ha in citrus; PRE at 1.8-10.8 kg ai/ha in grapes; PRE at 1.8-5.4 kg ai/ha in macadamia nuts; PRE at 2.2-4.5 kg ai/ha in papayas and ornamental trees; PRE at 0.9-4.5 kg ai/ha in peaches; PRE at 3.6-7.2 kg ai/ha in pineapple; PRE at 1.8-4.5 kg ai/ha in walnuts; and PRE at 3.6 kg ai/ha in ornamental bulbs. Diuron controls many annual weeds at lower rates and certain perennial weeds at higher rates.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable under normal storage conditions
Cleaning glassware/spray equipment: Flush equipment with water; clean glassware by washing with detergent followed by an acetone rinse
Emergency exposure: May irritate eyes, nose, throat, and skin
Incompatibilities: Compatible with most other herbicides; certain ester formulations of hormone weed killers may create a physical problem in the spray tank

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Foliar chlorosis concentrated around veins (sometimes interveinal) followed by necrosis
Absorption/translocation: Readily absorbed by roots, less so by foliage and stems; diuron is translocated rapidly from roots to shoots predominately by the xylem
Metabolism in plants: Differential metabolism via *N*-demethylation may be the basis for diuron selectivity (7). Demethylation is catalyzed in cotton by an *N*-demethylase (5). Diuron was metabolized to conjugates of monomethyl-diuron in *Torilis arvensis* and to *N*-dealkylated derivatives in *Lolium rigidum* (4).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Diuron resistance in *Chlamydomonas* (6) and kochia (9) was due to an altered site of action. Resistance to photosystem II inhibitors in rigid ryegrass was not caused by an alteration of the target site of these herbicides but appeared to be due to enhanced metabolism or sequestration of the herbicide within the leaves (3). Multiple resistance in annual ryegrass included resistance to diuron (2). Diuron resistance was found in *Amaranthus bouchonii* in Hungary (8).

BEHAVIOR IN SOIL

Sorption: Adsorbs to OM and clay

K_{oc}: Average is 480 mL/g (10)

Transformation:

Photodegradation: Not strongly photodegraded, but losses can be significant if diuron remains on the soil surface for several days or weeks

Other degradation: Microbial degradation is the primary means of diuron dissipation from soil.

Persistence: Average field half-life is 90 d (10). Phytotoxic residues dissipate within a season when applied at lower selective rates. At higher selective rates, residues may persist for more than 1 yr.

Mobility: Moderately leachable; leaching not a problem except on soils low in OM and clay

Volatilization: Probably insignificant losses except when diuron is exposed on the soil surface for several d or wk under hot, dry conditions

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade diuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 3400 mg/kg; Dermal LD_{50}, NA; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

KARMEX DF: Dermal LD_{50} rabbit, >2000 mg/kg

Subchronic toxicity:

90-d dietary, rat: NOEL 50-500 mg/kg

Chronic toxicity:

24-mo dietary, mouse: NOEL NA; increased mammary adenocarcinoma at 2500 mg/kg

24-mo dietary, rat: NOEL NA; malignant urinary bladder epithelium at 2500 mg/kg

24-mo dietary, dog: NOEL 125 mg/kg/d

Teratogenicity:

Rat: NOEL fetal 80 mg/kg/d, maternal 16 mg/kg/d; not teratogenic; body weight effects

Rabbit: NOEL fetal 50 mg/kg/d, maternal 10 mg/kg/d; not teratogenic.

Reproduction:

Rat: NOEL 250 mg/kg in a 2-generation study; not a reproductive toxin; body weight gain effects

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: *In vivo* cytogenetics, weakly clastogenic

DNA damage/repair: *In vivo* UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, 1730 mg/kg; Japanese quail 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck 8-d dietary $LC_{50,}$ >5000 mg/kg; Pheasant 8-d dietary $LC_{50,}$ >5000

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React 3,4-dichlorophenyl-isocyanate and dimethylamine

Purification of technical: Recrystallize 3 times from absolute ethanol

Analytical methods: Basic hydrolysis procedure for *p*-chloro compounds is applicable

Historical: First reported in 1951 (1). Introduced by DuPont Company; U.S. patent 2,655,445.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; Agriliance; BASF; Bayer CropScience; Drexel; DuPont; Crop Protection, Griffin; Helena; Micro Flo; Pro-Serve; Solvay Duphar; SSI Mobley; UAP-Platte; Wilbur-Ellis

Reference(s):

1. Bucha and Todd. 1951. Science 114:493.
2. Burnet, M. W. M. et al. 1991. Pages 427-428 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Ltd., Oxford.
3. Burnet, M. W. M. et al. 1991. Weed Sci. 39:317.
4. De Parado, R. et al. 1990. Weed Res. 30:213.
5. Frear, D. S. et al. 1969. Phytochemistry 8:2157.
6. Galloway and Mets. 1984. Plant Physiol. 74:469.

DSMA

disodium methylarsonate

CAS # DSMA: 144-21-8
Parent acid (MAA): 124-58-3

27$^{(Z)}$

NOMENCLATURE

Common name: DSMA (WSSA); MAA (WSSA) is the parent acid, methylarsonic acid

Other name(s): disodium methylarsonate (IUPAC); MAA = methylarsonic acid = parent acid of MSMA and DSMA; methylarsonic acid disodium salt

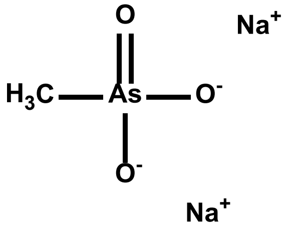
Trade name(s): ANSAR®; CALAR™; DSMA; SUMMER CRABICIDE®

Chemical family: arsenical; organic arsenical

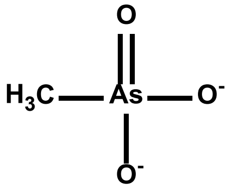
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

DSMA



MAA



Molecular formula: *DSMA*: $CH_3AsNa_2O_3$; *MAA*: CH_5AsO_3

Molecular weight: *DSMA*: 183.93 g/mole; *MAA*: 139.97 g/mole

Description: *DSMA and MAA*: White crystalline solid

Density: *MAA*: 0.95 g/mL; *DSMA 81 P*: 1.04 g/mL

Melting point: *DSMA 81 P (81% ai)*: 132-139 C; *MAA*: 161 C

Boiling point: NA

Vapor pressure: *DSMA*: 1.33×10^{-5} Pa (25 C); *MAA*: $>1 \times 10^{-5}$ Pa (25 C)

Stability: Stable at high and low temperature; stable under simulated sunlight

Solubility:

DSMA

water 269,000 mg/L (20 C)
organic solvents g/100mL:
n-hexane 0.00245
methanol 26

MAA

water 361,160 mg/L (25 C)

pK_a: 4.1 (1) and 8.94

K_{ow}: <10

HERBICIDAL USE

DSMA can be applied POST at 3.7 kg ai/ha in turf, POST at 2.5 kg ai/ha in cotton, and POST at 2.7-5.4 kg ai/ha in citrus and non-crop areas. Weeds controlled in turf include crabgrass spp., dallisgrass, and other grasses. DSMA also controls johnsongrass, nutsedge, foxtail spp., cocklebur, common ragweed, pigweed spp., and others. A surfactant is required for satisfactory efficacy. The Ca salt formulation of methanearsonate (CALAR) was developed because of greater turf tolerance than DSMA.

USE PRECAUTIONS

Fire hazard: All formulated products are dry or aqueous and nonflammable.

Corrosiveness: All formulated products are mildly corrosive.

Storage stability: All formulated products are completely stable. Solid formulations are somewhat hygroscopic and should be stored dry.

Cleaning glassware/spray equipment: Flush with water.

Emergency exposure: Wash eyes and skin with water for 15 min. If ingested, induce vomiting and lavage with water, followed by a saline cathartic, such as sodium sulfate. BAL (dimercaprol) is antidotal. Symptoms of mild poisoning include a salty taste, burning of throat, colicky stomach pains, and garlicky odor of breath or skin. Acute poisoning may occur with oral doses >30 g (1 oz) ai for an adult and symptoms include headache, vomiting, diarrhea, dizziness, stupor, convulsions, paralysis, and death.

Incompatibilities: Water high in Ca, Mg, and Fe may cause precipitation; these cations form insoluble methanearsonate salts.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood (2)

Symptomology: NA

Absorption/translocation: Only about 5% of DSMA absorbed by rice roots from nutrient solution translocated to the shoots (3).

Metabolism in plants: Rice roots and shoots slowly metabolize DSMA to the demethylated inorganic arsenic and to the methylated dimethyl and trimethyl arsenic species (3). Coastal bermudagrass and beans apparently do not cleave the C-As bond (4, 5).

Non-herbicidal biological properties: Some fungicidal action. See U.S. Patent 3,106,509. Ferric salts of methanearsonates have been used to control sheath blight of rice in Japan.

Mechanism of resistance in weeds: Organical arsenical-resistant cocklebur biotypes have been reported (6), but the mechanism of resistance is unknown.

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil

K_{oc}: Average is 7000 mL/g (estimated) (1)

Transformation: NA

Photodegradation: No losses

Persistence: Average field half-life is estimated at 180 d (1)

Mobility: NA

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with dry technical grade methylarsonic acid (MAA) unless otherwise indicated.

Acute toxicity:

DSMA 81 P: Oral LD_{50} rat, 1935 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 6 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, yes

Subchronic toxicity: NA

Chronic toxicity:

24-mo dietary, mouse: NOEL male 200 mg/kg, female 50 mg/kg; reduced body weight gain and increased water uptake at 400 mg/kg

12-mo dietary, dog: NOEL 2 mg/kg/d; diarrhea, vomiting, excessive salivation, and slightly decreased body weight at 35 mg/kg/d

Teratogenicity:

Rat: NOEL 10 mg/kg/d; slightly decreased food consumption and body weight gain at 100 mg/kg/d

Rabbit: NOEL 3 mg/kg/d; decreased food consumption and decreased body weight gain at 7 mg/kg/d

Reproduction:

Rat: NOEL maternal 7 mg/kg/d, developmental 22 mg/kg/d; reduced body weight in males at 76 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative with or without metabolic activation; Mouse lymphoma, negative with or without metabolic activation

Structural chromosome aberration: CHO, negative with or without metabolic activation

Wildlife:

DSMA 81 P: Bobwhite quail oral LD_{50}, 703 mg/kg, 8-d dietary LC_{50}, 4695 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Honey bee, relatively nontoxic; Daphnia 48-h LC_{50}, 153 mg/L; Bluegill sunfish 96-h LC_{50}, >112 mg/L; Rainbow trout 96-h LC_{50}, >114 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: DSMA ($CH_3AsO(ONa)_2$) synthesis involves two reactions:

$As_2O_3 + 6NaOH \rightarrow 2Na_3AsO_3 + 3H_2O$

$Na_3AsO_3 + CH_3Cl \rightarrow CH_3AsO(ONa)_2 + NaCl$

Also, see Initial Scientific Review of MSMA/DSMA, December 1975, U.S. Environmental Protection Agency, and references 5 and 6. U.S. patents 2,889,347, 2,695,306, and 2,442,372.

Purification of technical: Recrystallization from methanol.

Analytical methods: Titration with HCl, using an auto-end point titrometer. Total arsenic determination is done with sulfuric/nitric acid digestion followed by reduction with potassium iodide and subsequent titration with iodine to the starch-iodine blue endpoint. Atomic absorption spectrophotometry at 193.7 nm can be used. For residue methods, see Official Methods of Analysis, AOAC 12th ed., 25.006-25.013.

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Drexel; Helena; KMG Chemical; Lebanon; Luxembourg; Riverside/Terra; Setre Chemical; UAP-Platte

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Knowles and Benson. 1983. Plant Physiol. 71:235
3. Odanaka et al. 1985. J. Agric. Food Chem. 33:757.
4. Duble, R. L. et al. 1969. J. Agric. Food Chem. 17:1247.
5. Sachs and Michael. 1971. Weed Sci. 19:558.
6. Haigler, W. E. et al. 1988. Weed Sci. 36:24.

endothall

7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic

CAS # Diacid: 145-73-3
Dipotassium salt: 2164-07-0
Diammonium salt: 17439-94-0
Disodium salt: 129-67-9

NC

NOMENCLATURE

Common name: endothall (ANSI, WSSA).

Other name(s): endothal (BSI); endothal-sodium (ISO); ETH; 1,2-dicarboxy-3,6-*endo*-cyclohexane; 3,6-endoxohexahydrophthalic acid; 7-oxabicyclo[2.2.1] heptane-2,3-dicarboxylic acid (IUPAC)

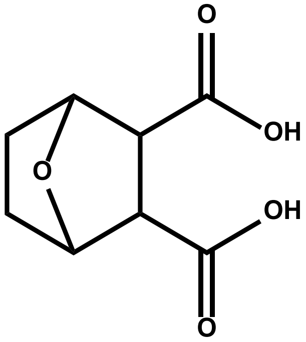
Trade name(s): ACCELERATE®; DES-I-CATE®; AQUATHOL®; AQUA THOL K; HERBICIDE 273; HYDROTHOL®; HYDROTHOL 191 GRANULAR; NIAGRATHAL; PENNOUT

Chemical family: None generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

endothall diacid



Molecular formula: *Diacid:* $C_8H_{10}O_5$; *Dipotassium salt:* $C_8H_8K_2O_5$; *Diammonium salt*: $C_{10}H_{16}N_2O_5$; *Disodium salt:* $C_8H_8Na_2O_5$

Molecular weight: *Diacid:* 186.16 g/mole; *Dipotassium salt:* 262.35 g/mole; *Diammonium salt:* 220.22 g/mole; *Disodium salt:* 230.13 g/mole

Description: White crystalline solid, odorless

Density: 1.431 g/mL

Melting point: 144 C

Boiling point: NA

Vapor pressure: NA

Stability: Stable to UV light; Slow conversion to the anhydride above ~90 C; Stable in acid

Solubility: water 100 g/L (pH 7, 25 C)

pK_a: 3.4 and 6.7 (1

K_{ow}: NA

HERBICIDAL USE

Endothall can be applied postplant incorporated at 3.36-7.4 kg ae/ha or POST at 0.84-1.68 kg ae/ha in sugarbeets to control several annual broadleaf and grass weeds including redroot pigweed, kochia, foxtail spp., barnyardgrass, and volunteer sunflowers. It also can be applied as a preharvest desiccant at 0.87-1.16 kg ae/ha in potatoes or at 0.6-0.87 kg ae/ha in alfalfa and clover seed crops. An oil adjuvant or diesel fuel may increase the rate and extent of potato vine desiccation.

Endothall can be sprayed or injected into ponds, lakes, and canals at 0.5-5 mg/L to control algae and several other aquatic weeds such as pondweed, burreed, milfoil, and coontail.

USE PRECAUTIONS

Fire hazard: All formulations are dry or aqueous and non-flammable.

Corrosiveness: Non-corrosive to metals

Storage stability: Stable to light. Liquid formulations should be stored above 0 C to prevent crystallization.

Cleaning glassware/spray equipment: Wash with water.

Emergency exposure: Potentially fatal if ingested; drink cold milk or cold water and call a doctor immediately. Flush eyes with water for at least 15 min; get immediate medical attention. Flush skin with water. Endothall concentrations over 1% produce a burning sensation on abraded skin.

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. In some plants, endothall inhibits lipid and protein biosynthesis (2). Its inhibitory effect on mRNA synthesis suggests action similar to that of actinomycin D (3). In other plant systems, endothall causes increased electrolyte leakage and increased levels of polyphenols followed by necrosis (4). Thus, endothall action may begin at the membranes.

Symptomology: Under both terrestrial and aquatic conditions, endothall symptoms are similar to those of chilling injury with defoliation and brown desiccated tissue. Endothall also inhibits root elongation when applied to the soil.

Absorption/translocation: Endothall rapidly penetrates the cuticle as the undissociated acid. It also is readily absorbed by plant roots. In turfgrass species, foliar- and root-applied endothall translocated primarily apoplastically (5). In other plant systems, movement in the apoplasm (including the xylem) was limited. Endothall can cause callose formation in the sieve tubes, which may account for its lack of phloem mobility. Injury is generally restricted to plant parts in contact with the herbicide.

Metabolism in plants: Endothall breaks down rapidly in water, but little is known of its metabolism in plants. Turfgrass plants treated with ^{14}C-endothall released $^{14}CO_2$ and produced an unidentified metabolite by 4 h after treatment (5).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 20 mL/g (estimated) at pH 7 (1). Ranges from 110-138 mL/g at pH 7.8

Transformation: Degraded by microbes in soil and water at rates varying with soil characteristics, temperature, and moisture

Persistence: Typical field half-life is 7 d (1), but half-life ranges from 3-7 d.

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade endothall diacid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 38-51 mg/kg; Dermal LD_{50}, NA; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

Endothall Na salt technical: Oral LD_{50} rat, 182-197 mg/kg

Endothall amine salt technical: Oral LD_{50} rat, 206 mg/kg

Subchronic toxicity: NA

Chronic toxicity:

24-mo dietary, rat: NOAEL >300 mg/kg

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife: NA

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Macro: gas chromatography. Micro: gas chromatography or flaxseed bioassay.

Historical: First reported in 1951 (6). Introduced by Sharples Chemical Corporation; U.S. patents 2,550,494, 2,576,080, and 2,576,081.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Cerexagri

Reference(s):

1. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
2. Corbett, J. R., K. Wright, and A. C. Baillie. 1984. The Biochemical Mode of Action of Pesticides, 2nd ed. Academic Press, New York.
3. Penner and Ashton. 1968. Weed Sci. 16:323.
4. Rikin and Rubin. 1983. Physiol. Plant. 59:161.
5. Turgeon, A. J. et al. 1972. Weed Sci. 20:557.
6. Tischler, N. et al. 1951. Proc. Northeast. Weed Control Conf. p. 51.

EPTC

S-ethyl dipropyl carbamothioate

CAS #: 759-94-4

8$^{(N)}$

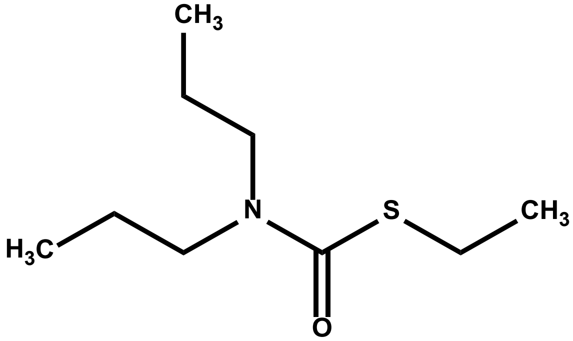
NOMENCLATURE

Common name: EPTC (BSI, ISO, WSSA)
Other name(s): S-ethyl dipropylcarbamothioic acid
Trade name(s): EPTAM® ; IMPERIUM®
Chemical family: Thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

EPTC



Molecular formula: $C_9H_{19}NOS$
Molecular weight: 189.32 g/mole
Description: Light yellow liquid, amine odor
Density: 0.96 g/mL (20 C)
Melting point: NA
Boiling point: 127 C (2.66 x 10^3 Pa)
Vapor pressure: 4.53 Pa (25 C)
Stability: Stable at < (200 C)
Solubility:
- water 370 mg/L (20 C)
- organic solvents (20 C):
- miscible in acetone, ethanol, kerosene, methylisobutylketone, 4-methylpentan-2-one, xylene

pK_a: None (non-ionizable)
K_{ow}: 1600

HERBICIDAL USE

EPTC can be applied to alfalfa, almonds, beans (green/dry), birdsfoot trefoil, citrus nursery stock and young field plantings (non-bearing orange and grapefruit groves), clovers, cotton, idle and fallow ground, lespedeza, pine seedling nurseries, potatoes, safflower, sugar beets, sunflower, tomatoes, and walnuts.

USE PRECAUTIONS

Fire hazard: EPTC technical is non-flammable; flash point is >93.3˚C. EPTAM 7E is non-flammable; flash point is 93.5˚C (closed cup).
Corrosiveness: Non-corrosive
Storage stability: Apparently indefinite storage life under normal ambient conditions**.**
Emergency exposure: Call a poison control center or physician immediately for treatment advice. Do not induce vomiting unless told to do so by a poison control center or physician.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Exerts its herbicidal action through inhibition of cuticle formation at the early stages of seedling growth. (more details on page 13)
Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Leaves are tightly rolled in the whorl and may not unroll normally. Injured dicot crops may have cupped or crinkled leaves with a thick, leathery texture. New leaves are puckered with a “drawstring effect”.
Absorption/translocation: Absorbed by roots and coleoptiles of emerging grass seedlings, although absorption by the coleoptile, especially near the coleoptilar node, is probably most important. Primary absorption in emerging susceptible broadleafs appears to occur in the hypocotyl hook.
Metabolism in plants: EPTC likely is oxidized to EPTC-sulfoxide or sulfone followed by reaction with glutathione (GSH). Metabolism of the GSH conjugate produced *N*-malonylcysteine conjugates.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds:
No known cases of resistance

BEHAVIOR IN SOIL

Sorption: EPTC is adsorbed onto dry soil. Adsorption increases as OM content increases.
Soil/Water Partition Coefficient: K_d/K_{oc} is 0.77 to 2.99/136 to 264, respectively.
Transformation: Primarily degraded by microbes
Persistence:
- **Field experiments:** Dissipation half-life in soil is 2-18.8 days (mean 8.6 days)
- **Lab experiments**: Metabolic half-life in soil is 13 to 28 days (aerobic conditions) and 31 to 127 days (anaerobic conditions).
- **Mobility**: Extent of leaching decreases as clay and OM content increases.
- **Volatilization**: Readily lost when the soil surface is moist at time of application and EPTC is not incorporated immediately.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.
Acute toxicity:
- Oral LD_{50} rat, 1465 mg/kg; male mouse, Dermal LD_{50} rabbit, >2000 mg/kg;; 4-h inhalation LC_{50} rat, 1.39 ppm; Skin irritation rabbit, mild-moderate; Skin sensitization guinea pig, weak; Eye irritation rabbit, mild

EPTAM 7-E: Oral LD_{50} rat, 1325-1500 mg/kg bw; Dermal LD_{50} (rabbit), 2750 mg/kg bw; Inhalation LC_{50} (rat), 4-h 10.3 mg/L air; Eye contact (rabbit), moderately irritating; Skin contact (rabbit), mildly irritating

Subchronic toxicity:

90-day oral rat: NOAEL 3mg/kg/day

90-day oral, dog: NOAEL15mg/kg/day

Chronic toxicity:

18-month oral, mouse: NOAEL 90 mg/kg/day; not oncogenic

24-month oral, rat: NOAEL 5 mg/kg/day; not oncogenic

12-month oral, dog: NOAEL 8 mg/kg/day

Teratogenicity:

Rat: NOAEL 100 mg/kg/day (maternal and development

Rabbit: NOAEL 40 mg/kg/day (maternal and development

Wildlife:

Bobwhite quail LC_{50}, 20000 mg a.i./kg-diet; Mallard duck, LD_{50}, >1000 mg a.i./kg-bw; Honey bee oral LD_{50}, >12.09 µg/bee; Bluegill sunfish 96-h LC_{50}, 14 mg/L; Water flea 48-h EC_{50}, 6.5 mg/L; Sheepshead minnow 96-h LC_{50}, 17 mg a.i./L; Eastern oyster 96-h EC_{50}, 1.8 mg a.i./L; White shrimp 48-h LC_{50}, 0.63 mg a.i./L; Green algae 4-d EC_{50}, 1.4 mg/L; Duckweed EC_{50}, 5.6 mg a.i./L

Mutagenicity: Weight of evidence from in-vitro tests and an in-vivo mouse micronucleus test indicate not mutagenic.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Ethyl chlorothiolformate is reacted with di-*n*-propyl amine and base.

Purification of technical: NA

Analytical methods: NA

Historical: Discovered in 1957 by Stauffer Chemical Co.; U.S. patent 2,913,327. EPTC was first reported in 1957 (1), and was introduced by Stauffer.

MANUFACTURER(S) AND INFORMATION SOURCES:

Manufacturer(s): Gowan Company

Source(s): Gowan Company

Reference(s):

1. Environmental Protection Agency (EPA). Reregistration Eligibility Decision (RED) for EPTC. December 1999.

esprocarb

CAS #: 85785-20-2 **8$^{(N)}$**

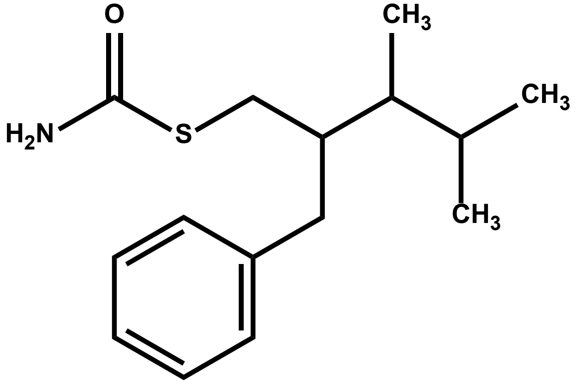
S-(phenylmethyl)(1,2-dimethylpropyl)ethylcarbamothioate

NOMENCLATURE

Common name: esprocarb (BSI, draft E-ISO; (m) draft F-ISO)
Other name(s): ICI-A2957; *S*-benzyl (*RS*)1,2-dimethylpropyl(ethyl)thiocarbamate (IUPAC)
Trade name(s): FUJIGRASS; SPARKSTAR, GAESENMOON (S.Korea)
Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
esprocarb



Molecular formula: $C_{15}H_{23}NOS$
Molecular Weight: 265.41 g/mole
Description: Translucent liquid
Density: 1.04 g/mL
Melting point: NA
Boiling point: 135 C (4.67 x 10^3 Pa)
Vapor pressure: 1.01 x 10^{-2} Pa (25 C)
Stability: Stable at 120 C; photolyzed in water DT_{50} 21 d (pH 7, 25 C)
Solubility:

water 4.9 mg/L (20 C)

ethanol	chlorobenzene
xylene	acetone

acetonitrile >1 g/kg (25 C)

pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 4.6

HERBICIDAL USE

Post-emergence control of annual weeds and *Echinochloa spp.* in paddy rice at 1.5-4 kg/ha; specifically developed for use in Japanese rice crops; may be applied any time from 5-15 d after transplanting; controls *Echinochloa* for up to 40 d.

USE PRECAUTIONS

Fire Hazard: Flash point = 100 C; combustion or thermal decomposition will evolve toxic and irritant vapors.
Corrosiveness: NA
Emergency exposure: If ingested, do not induce vomiting, wash mouth out with water and seek medical advice. On eye contact, rinse with water for 15 min.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)
Symptomology: NA
Absorption/translocation: NA
Metabolism in plants: NA
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: Evidence in soil
Other degradation: Slow degradation in soil
Persistence: Half-life in soil is 30-70 days
Mobility: Low
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade esprocard unless otherwise indicated.
Acute toxicity:
Female rat LD_{50}, 3700 mg/kg; Dermal rabbit LD_{50}, >2000 mg/kg; Rat LC_{50} inhalation (4 h), >4.06 mg/L in 4 h; Skin and eye irritation rabbit, mild; Skin sensitization guinea pigs, no
Subchronic toxicity: NA
Wildlife:
Japanese quail LD_{50}, >2000 mg/kg; Mirror carp LC_{50} (48 h), 1.52 mg/L
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: Discovered by Stauffer Chemical Co. it was first sold in 1987.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection
Reference(s):

1. Casida, J. E. et al. 1974. Science 184:573.
2. Fuerst, E. P. 1987. Weed Technol. 1:270-277.
3. Gronwald, J. W. 1991. Weed Sci. 39:435.
4. Prakash, T. R. et al. 1989. Weed Res. 19:427.

ethalfluralin

CAS #: 55283-68-6 **3$^{(K_1)}$**

N-ethyl-*N*-(2-methyl)-2-propenyl)-2,6-dinitro-4-(trifluoromethyl)benzenamine

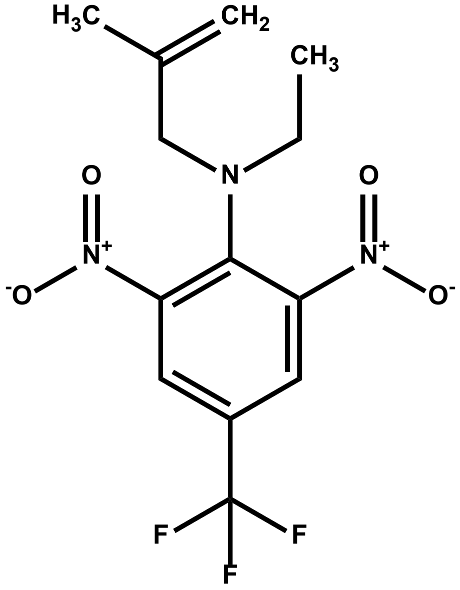
NOMENCLATURE

Common name: ethalfluralin (ANSI, BSI, ISO, WSSA)
Other name(s): ethalfluraline; ELI-161; *N*-ethyl-α,α,α–trifluoro-*N*-(2-methylallyl)-2,6-dinitro-*p*-toluidine (IUPAC)
Trade name(s): SONALAN®; EDGE®; CURBIT®; STRATEGY®
Chemical family: dinitroaniline

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

ethalfluralin



Molecular formula: $C_{13}H_{14}F_3N_3O_4$
Molecular weight: 333.27 g/mole
Description: Yellow-orange crystal, faint amine odor
Density: 1.32 g/mL
Melting point: 57-59 C
Boiling point: NA
Vapor pressure: 1.09 x 10^{-2} (25 C)
Stability: Degraded by UV light; degraded above 256 C
Solubility:
water 0.3 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C):
acetone >50 methanol 8.2-10
acetonitrile >50 methylene chloride >50
benzene >50 xylene >50
chloroform >50
pK_a: None (non-ionizable)
K_{ow}: 130,000 (pH 7, 25 C)

HERBICIDAL USE

Ethalfluralin can be applied PPI at 0.63-1.46 kg ai/ha in soybeans, 0.63-1.80 in sunflowers, and 0.63-1.34 in peanuts, PPI at 0.63-1.80 kg ai/ha in dry beans, and PPI at 1.26-1.80 kg ai/ha in pumpkin and squash. Ethalfluralin granules can be applied in standing wheat stubble and incorporated in late fall or early spring with conservation-till implements on land to be seeded to sunflowers, Ethalfluralin primarily controls annual grasses such as foxtail spp., barnyardgrass, fall panicum, and crabgrass spp. At medium to high rates, it also controls certain annual broadleaf weeds at such as redroot pigweed, Kochia, and black nightshade.

USE PRECAUTIONS

Fire hazard: Technical is non-flammable, ; flash point is 30 C; SONALAN HFP is non-flammable; flash point is 48.3 C
Corrosiveness: Non-corrosive
Storage stability: Shelf life of EC formulations is 2 yr. EC formulation should not be stored below 5 C
Cleaning glassware/spray equipment: Clean equipment with detergent and water
Emergency exposure: Wash skin with soap and water. Flush eyes with water and call a physician.
Incompatibilities: Compatible with hard water and other pesticides; no known incompatibilities

BEHAVIOR IN PLANTS

Mechanism of action: Mitotic disruption through inhibition of the microtubule protein tubulin (more details on page 12)
Symptomology: Most susceptible annual grasses and small-seeded broadleaf weeds fail to emerge, due to inhibition of coleoptile growth or hypocotyl unhooking. Seed germination is not inhibited. Root growth inhibition is a prominent symptom on emerged seedlings and established plants, especially in development of lateral and secondary roots. Roots appear stubby with tips becoming thickened. The stems of grasses such as corn may be purple near the base. The base of grass shoots swell, appearing bulbous, and the hypocotyl may swell in broadleaves. Shoots may be deformed and brittle.
Absorption/translocation: Absorbed primarily by emerging shoots (grass coleoptile, broadleaf hypocotyl or epicotyl), secondarily by seedling roots. Ethalfluralin vapors can be absorbed by the foliage and cotyledons (12). Although most dinitroaniline herbicides do not appear to translocate appreciably (3), 30% of absorbed ethalfluralin translocated to shoots of Solanum spp. (6), with similar results in cucumber seedlings (12). In the latter study, however, little translocated when the herbicide was applied to foliage. Thus, ethalfluralin apparently translocates to a moderate extent in the xylem, but movement in the phloem is minimal.
Metabolism in plants: Between 12 and 48% of applied ethalfluralin was converted to an unidentified water-soluble metabolite(s) by 24 h after application, with one additional methanol-soluble metabolite formed, and most ethalfluralin remaining unmetabolized in Solanum spp. (6). Ethalfluralin appears to be more rapidly metabolized than trifluralin. No significant levels of ethalfluralin metabolites have been detected in mature drybeans, soybeans, peanuts, or cotton.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Trifluralin-resistant goosegrass from the southern U.S. also is resistant to other dinitroaniline herbicides (2). The resistance mechanism may involve either a change in the binding site on tubulin subunits (8) or an altered microtubule-associated protein (9).

BEHAVIOR IN SOIL

Sorption: Adsorption of ethalfluralin was strong in all soil types tested, with K_{OC} values in the range 3967 to 8083 mL/g (average 5,000 mL/g) indicating that ethalfluralin will be 'non-mobile' in soil.

Transformation:

Photodegradation: Photolysis will contribute to the degradation of ethalfluralin in soil.

Other degradation: Ethalfluralin steadily degrades in soil under aerobic conditions in the laboratory, with DT_{50} values ranging from 24 to 47 days. The overall mean DT_{50} value across four soils is 34 days..

Persistence: Dissipation in the field was overall slightly slower than that observed under laboratory conditions, This is considered to be due to the lower overall temperature involved outdoors and the incorporation of ethalfluralin in the soil following application (which will reduce volatilization losses). Soil dissipation studies show that the DT_{90} (field) value of ethalfluralin in southern Europe is < 1 year (range 71 to 347 days, mean 177 days) and, therefore, ethalfluralin has no potential to accumulate in soil following successive applications.

Mobility: Negligible leaching

Volatilization: Low but significant losses if allowed to remain on the soil surface for several days under warm, moist conditions

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade ethalfluralin unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5,000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50}, >0.94 mg/L; Skin irritation rabbit, moderate to severe; Skin sensitization guinea pig, yes; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, mouse: NOEL 68 mg/kg/d;

90-d dietary, rat: NOEL 29 mg/kg/d

90-d dietary, dog: NOEL 27.5 mg/kg/d

Chronic toxicity:

18-mo dietary mouse: NOEL 10.3 mg/kg/d; no evidence of carcinogenicity up to the highest dose tested, 163 mg/kg/d

24-mo dietary, rat: NOEL 32.2 mg/kg/d;

Evidence of oncogenicity (increased incidence of benign mammary fibroadenomas at mid (10.7 mg/kg/d) and high doses (32.3 mg/kg/d). EPA classifies ethalfluralin as a Class C carcinogen (Possibly carcinogenic to humans: agents with limited animal evidence and little or no human data).

12-mo dietary, dog: NOEL 4 mg/kg/d; minor effects at up to 80 mg/kg/d

Teratogenicity:

Rat: Developmental NOEL 1000 mg/kg/d (HDT)

Rabbit: Developmental NOEL 75 mg/kg/day

Reproduction:

Rat: No abnormalities in r offspring and no reproductive effects up to the highest dose tested, reproductive NOEL ≥61 mg/kg/d

Mutagenicity: Negative for several tests

Gene mutation: Ames test, weakly positive. In vitro mammalian chromosome aberration assay in CHO: negative without S9 activation and positive with activation.

Wildlife:

Northern bobwhite acute oral LD_{50}, >2000 mg/kg; Northern bobwhite 8-d dietary LC_{50}, >5000 mg/kg; mallard duck 8-d dietary LC_{50}, >5000 mg/kg; rainbow trout 96-h LC_{50}, = 0.136 mg/L; bluegill 96-h LC_{50}, = 0.102 mg/L; Daphnia 48-h EC_{50}, >0.0060 mg/L; honeybee 48-h contact LD_{50}, = 51 µg/bee; earthworm 14-d LC_{50}, >103 mg/kg; green algae 96-h EC_{50}, = 0.025 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Nitration (in the presence of nitric acid and sulfuric acid) of 4-trifluoromethyl-1-chlorobenzene yields the 2,6-dinitro derivative; subsequent treatment with *N*-ethyl-*N*-(2-methyl-2-propenyl) amine produces ethalfluralin

Purification of technical: Dissolve crude mixtures in hexane and pass over a Florisil chromatographic column. Further purification is done by recrystallization from hexane or ethanol.

Analytical methods: Formulated products are extracted with chloroform and the resulting solution analyzed by GC using flame ionization detection. Crop tissue or soil is extracted with methanol or acetonitrile, cleaned up on a Florisil column, and determined by GC using electron capture detection. Assay sensitivity is 5-10 □g/kg.

Historical: First described as herbicide in 1974 (5). SONALAN HFP was introduced in 1994.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Dow AgroSciences; UAP-Platte

Reference(s):

1. Mudge, L. C. et al. 1984. Weed Sci. 32:591.
3. Penner, D. 1971. Weed Sci. 19:571.
4. Skylakakis, G. et al. 1974. Proc. 12th Br. Weed Control Conf. 12:795.
6. USA EPA Registration Eligibility Decision (RED). Ethalfluralin, March 1995, EPA 738-R-95-001.
7. Vandeventer, J. W. et al. 1986. Pestic. Sci. 17:380.
8. Vaughan, K. C. et al. 1987. Plant Physiol. 83:956.
9. Vaughan, K. C. et al. 1990. Weed Technol. 41:157.
10. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
12. Willis and Putnam. 1985. Weed Sci. 34:13.

ethametsulfuron-methyl

CAS #: 97780-06-8

$2^{(B)}$

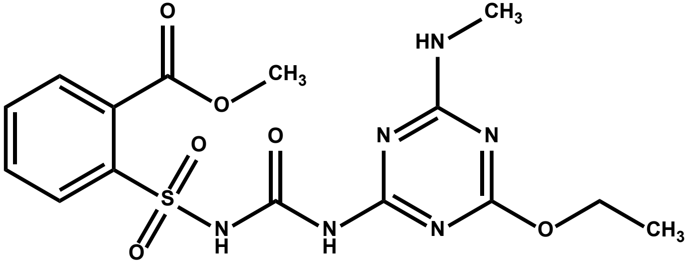
methyl 2-[[[[4-ethoxy-6-(methylamino)-1,3,5-triazin-2-yl] amino]carbonyl]amino]sulfonyl]benzoate

NOMENCLATURE

Common name: ethametsulfuron-methyl (ANSI, BSI, ISO, WSSA)
Other name(s): DPX-A7881; methyl 2-[(4-ethoxy-6-methylamino-1,3,5-triazin-2-yl)carbamoylsulfamoyl] benzoate (IUPAC)
Trade name(s): MUSTER®
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
ethametsulfuron-methyl



Molecular formula: $C_{15}H_{18}N_6O_6S$
Molecular weight: 410.40 g/mole
Description: White crystalline solid
Density: NA
Melting point: 194 C
Boiling point: NA
Vapor pressure: 7.7 x 10^{-13} Pa (25 C)
Stability: NA
Solubility:
water 1.7 mg/L (pH 5); 50 mg/L (pH 7); 410 mg/L (pH 9)
organic solvents g/100 mL:
acetone 0.16
acetonitrile 0.083
ethanol 0.017
ethyl acetate 0.069
n-hexane < 0.0005
methanol 0.0035
methylene chloride 0.39
toluene 0.0009
xylenes 0.001
pK_a: 4.6 (weak acid)
K_{ow}: 0.89 (pH 7)

HERBICIDAL USE

Ethametsulfuron can be applied POST at 20-30 g ai/ha in spring canola (rapeseed) for control of certain broadleaf weeds such as wild mustard, hempnettle, green smartweed, and stinkweed.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Cleaning glassware/spray equipment: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: NA
Absorption/translocation: NA
Metabolism in plants: Excised shoots of canola metabolized a transpired pulse of ethametsulfuron-methyl with DT_{50} of 5-14 h (2). Metabolism of ethametsulfuron-methyl in canola via foliage treatment involved the dealkylation of the *O*- and *N*- substituents at the triazine moiety.
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Persistence: NA
Mobility: NA
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade ethametsulfuron acid unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, > 5000 mg/kg; Dermal rabbit LD_{50}, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.7 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild
MUSTER: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none
Subchronic toxicity:
90-day dietary, mice: NOEL 5000 mg/kg/d
90-day dietary, dog: NOEL 10,000 mg/kg
Chronic toxicity:
18-mo dietary, mouse: NOEL 5000 mg/kg; not oncogenic
24-mo dietary, rat: NOEL 500 mg/kg; not oncogenic; serum sodium effects at 5000 mg/kg
12-mo dietary, dog: NOEL 3000 mg/kg; effects on hematology parameters at 15,000 mg/kg
Teratogenicity:
Rat: NOEL 1000 mg/kg/d; not teratogenic; fetal weight effects at 4000 mg/kg/d
Rabbit: NOEL 250 mg/kg/d; not teratogenic; maternal effects at 1000 mg/kg/d, and fetal effects at 4000 mg/kg/d
Reproduction:
Rat: NOEL 5000 mg/kg; body weight effects at 20,000 mg/kg
Mutagenicity:
Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: *In vito* cytogenetics, negative; Mouse micronucleus, negative

DNA damage/repair: Rat hepatocytes/ UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >5620 mg/L; Mallard duck oral LD_{50}, >2250 mg/kg, 8-d dietary LC_{50}, >5620 mg/L; Earthworm LC_{50}, >1000 mg/kg; Honey bee LD_{50}, >12.5 µg/bee; Daphnia 48-h LC_{50}, > 550 mg/L; Bluegill sunfish 96-h LC_{50}, >600 mg/L; Rainbow trout 96-h LC_{50}, >600 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

ethofumesate

CAS #: 26225-79-6 **$8^{(N)}$**

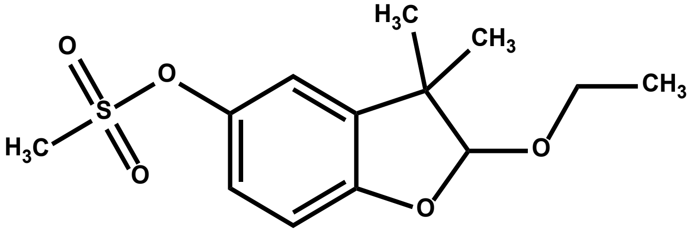
2-ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate

NOMENCLATURE

Common name: ethofumesate (ANSI, BSI, ISO, WSSA)
Other name(s): NC 8438; (*RS*)-2-ethoxy-2,3-dihydro-3,3-dimethylbenzofuran-5-yl methanesulfonate (IUPAC)
Trade name(s): BETAMIX PROGRESS™; GALAHAD®; GREENCLENE; MAGIC TANDEM®; MORLEX; NEW MURBETEX; NORTON® SC; PROGRASS™; PROGRESS®; PROGRESS® BETA; TRAMAT®
Chemical family: benzofuranes; benzofuranyl alkylsulfonate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
Ethofumesate



Molecular formula: $C_{13}H_{18}O_5S$
Molecular weight: 286.34 g/mole
Description: White crystalline solid, odorless
Density: 0.95 g/mL
Melting point: 70-72 C
Boiling point: NA
Vapor pressure: 8.60 x 10^{-5} Pa (25 C)
Stability: Stable to UV light
Solubility:
water 110 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 40
benzene 40
chloroform 40
dioxan 40
ethanol 10
glycerol 25
n-hexane 0.04
pK_a: None (non-ionizable)
K_{ow}: 501 (25 C)

HERBICIDAL USE

Ethofumesate can be applied before or after weed emergence at 0.84-2.1 kg ai/ha in grass seed and sod, and applied PPI or postplant incorporated at 2.24-4.2 kg ai/ha in sugarbeets (incorporation before planting not required in sprinkler-irrigated sugarbeets). Weeds controlled include black nightshade, common chickweed, lambsquarters, kochia, redroot pigweed, Russian thistle, wild buckwheat, barnyardgrass, large crabgrass, foxtail spp., downy brome, and soft chess.

USE PRECAUTIONS

Fire hazard: NORTRON EC is flammable; flash point is 29.4 C using Abel/Pensky Martin closed cup method
Corrosiveness: NORTRON EC is non-corrosive
Storage stability: NORTRON EC has an indefinite stability if protected from frost.
Cleaning glassware/spray equipment: Rinse with water and detergent
Emergency exposure: Flush eyes and skin with water for at least 15 min. Consult a physician in case of eye exposure. If NORTRON SC is ingested, drink 1-2 glasses of water and induce vomiting.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Appears to be inhibition of lipid synthesis at a site other than ACCase. (more details on page 13)
Symptomology: NA
Absorption/translocation: Readily absorbed by emerging shoots (grass coleoptile and broadleaf hypocotyl) and roots, and translocated readily to the foliage. POST-applied ethofumesate is poorly absorbed by maturing leaves with a well-developed cuticle.
Metabolism in plants: Ryegrass and tolerant sugarbeets produce two conjugated metabolites, one major and one minor.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: Average is 340 mL/g (2)
Transformation:
Photodegradation: Negligible losses
Other degradation: Microbially degraded in soil
Persistence: Half-life ranges from >14 wk under dry, cold conditions to <5 wk under warm, moist conditions.
Lab experiments: Activity of ethofumesate applied at 1 or 3 mg/kg was reduced 90% after 14 wk in a coarse sandy loam and in an organic clay soil under warm, moist conditions.
Mobility: Little leaching in soils with >1% OM. Ethofumesate is not readily leached below 15 cm (6 inches).
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade ethofumesate unless otherwise indicated.

Acute toxicity: Oral LD_{50} rat, <6400 mg/kg; Dermal LD_{50} rabbit, <20,050 mg/kg; 6-h inhalation LC_{50} rat, >0.5 mg/L; Skin irritation rabbit, slight; Skin sensitization, NAv; Eye irritation rabbit, slight
Subchronic toxicity:
90-d dietary, rat: NOEL NA; no effects at 400 ppm.

Chronic toxicity:

24-mo dietary, rat: NOEL >1000 mg/kg/d

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail, oral LD_{50}, >8743 mg/kg, 5-d dietary LC_{50}, >10,000 mg/kg; Mallard duck, oral LD_{50}, <3552 mg/kg, 5-d dietary LC_{50}, >10,000 mg/kg; Japanese quail LD_{50}, >1600 mg/kg; Honey bee, nontoxic; Daphnia 48-h LC_{50}, 295 mg/L; Bluegill sunfish 96-h LC_{50}, <320 mg/L; Guppy 24-h LC_{50}, 15 mg/L; Rainbow trout 96-h LC_{50}, <180 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Reaction of the enamine from morpholine and 2-methyl propionaldehyde with *p*-benzoquinone to give 2,3-dihydro-3,3-dimethyl-2-morpholinobenzo-furan-5-ol which is mesylated and the product converted to ethofumesate.

Purification of technical: Recrystallization from ethanol.

Analytical methods: Consult Analytical Methods for Pesticides and Plant Growth Regulators, 1978, Academic Press.

Historical: Herbicidal properties first described in 1969 (1); protected by U.S. patent 3,689,507 and British patent 1,271,659

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Pfeiffer, R. K. 1969. 3rd Symp. New Herbicides. E.W.R.C. Paris, p. 1.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

ethoxysulfuron

CAS #: 126801-58-9

$2^{(B)}$

2-ethoxyphenyl [[(4,6-dimethoxy-2-pyrimidinyl)amino]
carbonyl]sulfamate

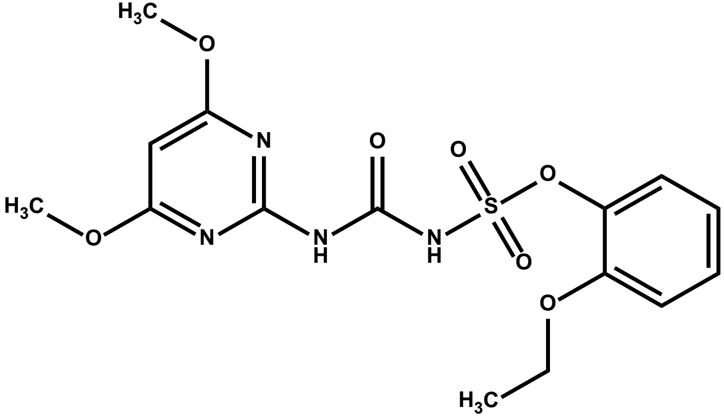
NOMENCLATURE

Common name: ethoxysulfuron (ISO-approved)
Other name(s): HOE 095404; HOE-404; 1-(4,6-dimethoxypyrimidin-2-yl)-3-(2-ethoxyphenoxysulfonyl)urea (IUPAC)
Trade name(s): GLADIUM®; GRAZIR; HERO®; RICESTAR®; SKOL®; SUNRICE®; SUNSTAR®; TILLER®; XTRA
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

ethoxysulfuron



Molecular formula: $C_{15}H_{18}N_4O_7S$
Molecular weight: 398.39 g/mole
Description: White to beige powder
Density: NA
Melting point: 144-147 C
Boiling point: Decomposes before reaching boiling point
Vapor pressure: 6.62×10^{-5} Pa (20 C); 1.2×10^{-4} Pa (25 C); Henry's Law constant, 1.94×10^{-3} P m^3mol^{-1} (pH 7, 20 C)
Stability: Hydrolytic DT_{50} 65 d (pH 5); 259 d (pH 7); 331 d (pH 9)
Solubility:
water 5.5 mg/L (pH 3); 1353 mg/L (pH 7); 5452 mg/L (pH 10)
organic solvents g/L:

acetone 36.0	methanol 7.7
dichloromethane 107	isopropanol 1.0
toluene 2.5	ethyl acetate 14.1
n-hexane 0.006	

pK_a: 5.28 (weak acid)
K_{ow}: log K_{ow} = 2.89 (pH 3); 0.004 (pH 7)

HERBICIDAL USE

Ethoxysulfuron is used for broadleaf and sedge weed control in cereals, rice, and sugarcane at rates of 10-120 g a.i./ha. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Non-corrosive
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 11)
Symptomology: Chlorosis of young foliage followed by necrosis and plant death.
Absorption/translocation: Absorbed by roots and leaves; translocated primarily by the phloem
Metabolism in plants: NA
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: Altered site of action

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Persistence:
Field experiments: DT_{50} 18-20 d; in paddy conditions DT_{50} 10-60 d
Volatilization: Not volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade ethoxysulfuron unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 3270 mg/kg; Dermal LD_{50} rat, >4000 mg/kg; non-irritating to skin or eyes
Mutagenicity: Non-mutagenic
Wildlife: NA
Use classification: WHO Class III

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

fenchlorazole-ethyl

CAS #:103112-35-2

NC

ethyl 1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1*H*-1,2,4-triazole-3-carboxylate

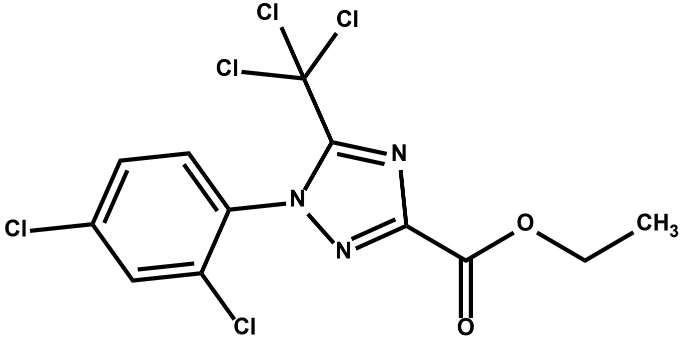
NOMENCLATURE

Common name: fenchlorazole-ethyl (ISO)
Other name(s): HOE-70542; ethyl 1-(2,4-dichlorophenyl)-5-trichloromethyl-1*H*-1,2,4-triazole-3-carboxylate (IUPAC)
Trade name(s): TRISTAR®
Chemical family: triazole carboxylate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

fenchlorazole-ethyl



Molecular formula: $C_{12}H_8Cl_5N_3O_2$
Molecular weight: 403.48 g/mole
Description: White solid
Density: NA
Melting point: 108-112 C (technical)
Boiling point: NA
Vapor pressure: 8.9×10^{-9} Pa (20 C)
Stability: Stable
Solubility:
  water 0.9 mg/L (20 C)
  organic solvents g/L (20 C):
  acetone - 360
  dichloromethane - > 500
  n-hexane - 2.5
  methanol - 27
  toluene - 370
pK$_a$: NA
K$_{ow}$: NA

HERBICIDAL USE

Fenchlorazole-ethyl is a herbicide safener used in Europe and Canada to protect wheat, durum wheat, rye, and triticale against injury from the aryloxyphenoxypropionate herbicide fenoxaprop (1). The safener is not registered for use in the US.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent.
Emergency exposure: If on skin, wash with plenty of soap and water. Get medical attention if irritation persists. If in eyes, flush with plenty of water. Call a physician if irritation persists. If inhaled, remove victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: When applied in combination with fenoxaprop, fenchlorazole-ethyl prevents growth retardation, leaf discoloration, and chlorosis of the crop, which is usually visible within a few days if fenoxaprop is sprayed alone. Fenchlorazole-ethyl accelerates the metabolic breakdown of fenoxaprop in wheat and the formation of non-phytotoxic metabolites (2, 3). Fenchlorazole-ethyl does not reduce the herbicidal activity of fenoxaprop on target grass weeds. On the contrary, the safener appears to act as a synergist enhancing the efficacy of fenoxaprop on selected grass weeds such as crabgrass (3).
Symptomology: Fenchlorazole-ethyl applied by itself either PRE or POST does not show any herbicidal activity. Under greenhouse conditions and at high rates of up to 10 kg ai/ha, no herbicidal effects were observed on eight broadleaf, grass, and sedge weed species. No symptoms are visible since the compound is not phytotoxic.
Absorption/translocation: Generally absorbed rapidly by the roots and foliage of winter cereals.
Metabolism in plants: NA
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: None known

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Persistence: NA
Mobility: NA
Volatilization: Non-volatile
Formulation effects: Environmental fate properties are unaffected by formulation type.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fenchlorazole-ethyl.

Acute toxicity:

Oral LD$_{50}$ rat, > 5000 mg/kg; mouse, >2000 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; rat, >2000 mg/kg; Primary eye irritation rabbit, negative; Skin irritation rabbit, negative; Skin sensitization guinea pig, negative

Subchronic toxicity:

90-d dietary, mouse: 80 mg/kg/d (males); 320 mg/kg/d (females)
90-d dietary, rat: 1280 mg/kg/d
90-d dietary, dog: 80 mg/kg/d

Chronic toxicity:
12-mo dietary, dog: 80 mg/kg/d
Teratogenicity:
Rat: Not teratogenic
Rabbit: Not teratogenic
Reproduction: NA
Mutagenicity: Not mutagenic
Wildlife: Studies showed that this safener is not acutely toxic to wildlife mammals, has low toxicity to birds, is not toxic to bees and has negligible effects on soil microorganisms.
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: Chromatographic methods (TLC, GC, and HPLC) are available. Contact Bayer for details.
Historical: This safener was introduced by Hoechst in 1989. It is used in combination with fenoxaprop for winter cereal production in Europe.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1. Bieringer, H. et al. 1989. Proc. Brighton Crop Prot. Conf.-Weeds, pp. 77-82.
2. Kocher, H. et al. 1989. Proc. Brighton Crop Prot.. Conf.-Weeds, pp. 495-500.
3. Yaacoby, T et al. 1991. Pestic. Biochem. Physiol. 41: 296.

fenclorim

4,6-dichloro-2-phenyl-pyrimidine

CAS #: 3740-92-9

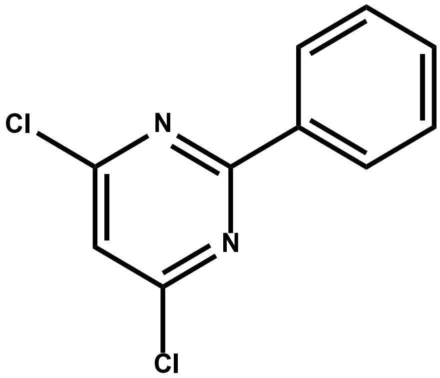
NC

NOMENCLATURE

Common name: fenclorim (ISO)
Other name(s): CGA-123407; 4,6-dichloro-2-phenylpyrimidine (IUPAC)
Trade name(s): SOFIT
Chemical family: pyrimidine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
fenclorim



Molecular formula: $C_{10}H_6Cl_2N_2$
Molecular weight: 225.08 g/mole
Description: Odorless, colorless crystalline solid
Density: 1.5 g/mL (20 C)
Melting point: (96.9 C)
Boiling point: NA
Vapor pressure: 1.2×10^{-2} Pa (20 C); 4.6×10^{-2} Pa (30 C); 1.6×10^{-1} Pa (40 C)
Stability: Stable up to (400 C)
Solubility:
- water 2.5 mg/L (20 C)
- organic solvents (20 C):
- methanol - 1.9%
- isopropanol - 1.8%
- n-octanol - 4.2%
- acetone - 14%
- cyclohexanone - 28%
- methylene chloride - 40%
- xylene - 30%
- toluene - 35%
- hexane - 4%

pK_a: NA
K_{ow}: log K_{ow} = 4.17

HERBICIDAL USE

Fenclorim is a herbicide safener protecting rice against injury from the chloroacetanilide herbicide pretilachlor.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent soap and water. Get medical attention if irritation persists. If in eyes, flush with plenty of water. Call a physician if irritation persist. If inhaled, remove victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Enhances the activity of glutathione *S*-transferase (GST) enzymes in rice, which catalyze the conjugation of pretilachlor with glutathione (2, 3).
Symptomology: No symptoms are visible since the compound is not phytotoxic.
Absorption/translocation: Generally absorbed rapidly by rice roots (1)
Metabolism in plants: Fenclorim is metabolized in plants by conjugating to glutathione (2).
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: None known

BEHAVIOR IN SOIL

Sorption: NA
Transformation:

Photodegradation: Minor route of degradation. Only 9% of the parent decomposed in distilled water when exposed to light from xenon arc lamp filtered through borosilicate glass for 2 hours

Other degradation: The compound is susceptible to pH-dependent hydrolysis. The half-life at pH 9.0 and 70 C was 26 h.

Persistence: NA
Mobility: NA
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fenclorim unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >2500 mg/kg; Dermal LD_{50} rabbit, >4000 mg/kg; 4-h inhalation LC_{50} rat, >6.3 mg/L; Primary eye irritation rabbit, moderately irritating; Skin irritation rabbit, negative; Skin sensitization guinea pig, negative

Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA**Reproduction:** NA
Mutagenicity: NA
Wildlife: NA
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: Synthesis during manufacturing

results in technical active ingredient with a purity > 99%. No additional purification is needed.

Analytical methods: Chromatographic methods (TLC, GC, and HPLC) are available. Contact Novartis Crop Protection, Inc. for details.

Historical: This safener was introduced by Ciba-Geigy in 1983. It is used in combination with pretilachlor in many rice producing countries of Asia.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Christ, R.A. 1985. Weed Res. 5: 193.
2. Ebert, E. and H.R. Gerber. 1989. Pages 177-193 in Hatzios, K.K. and R.E. Hoagland (eds.). Crop Safeners for Herbicides. Academic Press.
3. Wu, J. et al. 1996. Pestic. Biochem. Physiol. 54:220.

fenoxaprop-P

CAS # Acid: 113158-40-0
Ethyl ester: 71283-80-2

$1^{(A)}$

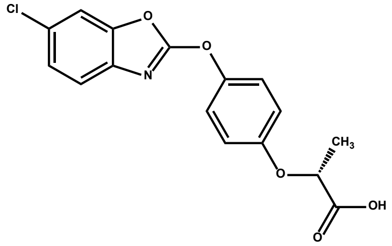
(2R)-2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]propanoic acid

NOMENCLATURE

Common name: fenoxaprop (ANSI, BSI, ISO, WSSA) for the racemic mixture of R and S isomers; fenoxaprop-P (BSI, ISO) for the R isomer
Other name(s): HOE-33171; HOE-46360; (Acid) (R)-2-[4-(6-chloro-1,3-benzoxazol-2-yloxy)phenoxy]propionic acid (IUPAC); (Ethyl ester) fenoxaprop-P ethyl = ethyl (2R) 2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]propanoate (CAS); ethyl (R)-2-[4-(6-chloro-1,3-benzoxazol-2-yloxy) phenoxy]propionate (IUPAC)
Trade Name(s): BAGHERA®; CHEETAH®; DOPLER®; FURORE®; FOXFIRE®; KENDO®; MAEDUSI; PARITY®; PODIUM® ; PUMA®POWER; PUMA® SUPER; RICESTAR®; RUMPAS®; STARICE®; TILLER®; WILDCAT®; WHIP®
Chemical family: aryloxyphenoxy propionate; aryloxyphenoxy propionic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: fenoxaprop-P acid



Molecular Formula: Acid $C_{16}H_{12}ClNO_5$; Ethyl ester $C_{18}H_{16}ClNO_5$
Molecular weight: Acid 333.73 g/mole; Ethyl ester 361.78 g/mole
Description: Beige to brown coarse powder, weakly aromatic
Density: 1.3 g/mL (20 C)
Melting point: 89-91 C
Boiling point: 300 C (1.33 x 10^{1} Pa)
Vapor pressure: 1.9 x 10^{-5} Pa (20 C); 4.3 x 10^{-6} Pa (25 C)
Stability: Slowly degraded by UV light; decomposed by acids and alkalis
Solubility:
water 0.5-1 mg/L (20 C)
organic solvents g/100 mL (20 C)
acetone 51 ethyl acetate 24
ethanol 2 n-hexane 0.5
pK_a: Acid NA; Methyl ester None
K_{ow}: 13,200

HERBICIDAL USE

Fenoxaprop-P can be applied POST at 37.5-111 g ai/ha in soybeans, POST at 0.04-0.39 kg ai/ha in turf, POST at 32.8-91.5 g ai/ha in wheat, and POST at 70.4-93.8 g ai/ha in conservation reserve (set-aside) land. Fenoxaprop rates are twice those of fenoxaprop-P. Fenoxaprop applied by itself is phytotoxic to wheat but has selectivity in wheat (excluding Durum) when applied with certain broadleaf herbicides (2,4-D, MCPA, thifensulfuron, and tribenuron) that antagonize its activity against wheat. The antagonism-based selectivity in wheat is utilized in the product TILLER. Fenoxaprop controls nearly all annual and some perennial grass weeds with no injury to broadleaf species.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Non-corrosive
Storage stability: Stable for >2 yr; do not store below -7 C
Cleaning glassware/spray equipment: Wash with detergent or approved spray tank cleaners
Emergency exposure: Flush eyes and skin with water for at least 15 min. If ingested, do not induce vomiting; seek immediate medical attention.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)
Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop within 1-3 wk of application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.
Absorption: The ethyl ester of fenoxaprop is rapidly absorbed into leaves and appears to be rainfast within about 2 h (2). Fenoxaprop ester readily diffuses across the plasmalemma. Once inside the cell, the ester is rapidly hydrolyzed to fenoxaprop acid which remains dissociated as the anion in the relatively alkaline cytoplasm. Because of its low lipophilicity, the polar fenoxaprop anion is largely prevented from diffusing back out across the plasmalemma. Fenoxaprop ethyl ester that is deesterified before entering the cell would tend to diffuse across the plasmalemma as the protonated fexoxaprop acid would (relatively lipophilic). Inside the phloem cells, fenoxaprop acid would dissociate to the anion, thereby trapping the herbicide in the phloem.
Translocation: Fenoxaprop predominately translocated in the phloem. Foliar-applied fenoxaprop accumulates in meristematic regions, although translocation rates are low and only about 2% of the absorbed fenoxaprop moves out of the treated leaf.
Metabolism in plants: Fenoxaprop ethyl ester is rapidly deesterified in plants to the herbicidally-active fenoxaprop acid. Further metabolism of the herbicide appears to be considerably slower than that of other aryloxyphenoxy propionate herbicides. Fenoxaprop ethyl ester applied

to wheat, barley, and crabgrass was metabolized 29, 63, and 9%, respectively, to products other than fenoxaprop acid 48 h after treatment (7). Following hydrolysis to fenoxaprop acid, the major metabolites include hydroxylated and nonhydroxylated benzoxazolone (6-chloro-2,3-dihydro-benzoxazol-2-one) and unidentified water-soluble metabolites which may be carbohydrate conjugates (6). The proportion of these major metabolites varies with species. Fenoxaprop tolerance among species generally is associated with higher rates of detoxification (4). At harvest, soybean seed were free of fenoxaprop or its metabolites.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Fenoxaprop-resistant biotypes of wild oats and green foxtail have been reported, but no mechanism has yet been determined.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 9490 mL/g for fenoxaprop ethyl ester (5).

Transformation: Under aerobic or anaerobic conditions, the half-life is <1 d for conversion of fenoxaprop ethyl ester to the phytotoxic fenoxaprop acid. The acid is degraded primarily to 6-chloro-2,3-dihydrobenzoxazole-2-one and 4-(6-chloro-2-benzoxazolyloxy)phenol.

Persistence: Typical half-life is 9 d (5-14 d depending on sol characteristics) under aerobic and 30 d under anaerobic condtions.

Photodegradation: Not a major pathway of degradation from soil surfaces.

Mobility: Low mobility in two silt loam soils and one silty clay soil. Residues have not been detected below 15 cm in soil. Aged residues of fenoxaprop also show no leaching potential.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fenoxaprop ethyl ester unless otherwise indicated.

Acute toxicity: Oral LD_{50} male rat, 3310 mg/kg, female rat 3400 mg/kg; Dermal LD_{50} male rabbit, >2000 mg/kg; 4-h inhalation LC_{50} *rat, 3.92 mg/L;* Skin irritation rabbit, slight; Skin sensitization, NA; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, rat: NOEL 80 mg/kg/d

90-d dietary, dog: NOEL 16 mg/kg/d

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail oral LD_{50}, >2510 mg/kg; Honey bee oral LD_{50}, >0.02 µg/bee; Daphnia 48-h LC_{50}, 11.15 mg/L; Bluegill sunfish 96-h LC_{50}, 3.34 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Details of HPLC methods are available from Bayer CropScience.

Historical: Fenoxaprop ethyl ester was introduced by Hoechst AG and first reported in 1982 (1).

MANUFACTURER(S) AND INFORMATION SOURCES

Industry source(s): Bayer CropScience

Reference(s):

1. Bieringer, H. et al. 1982. Proc. Br. Crop Prot. Conf.-Weeds 1:11.
2. Bryson, C. T. 1988. Weed Technol. 2:153.
3. Kobek, K. et al. 1988. Z. Naturforsch. 43c:47.
4. Lefsud and Hall. 1989. Pestic. Biochem. Physiol. 34:218.
5. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
6. Wink, O. et al. 1984. J. Agric. Food Chem. 32:187.
7. Yaacoby, T. et al. 1991. Pestic. Biochem. Physiol. 41:296.

fentrazamide

CAS #: 158237-07-1

$15^{(K_3)}$

4-(2-chlorophenyl)-*N*-cyclohexyl-*N*-ethyl-4,5-dihydro-1*H*-tetrazole-1-carboxamide

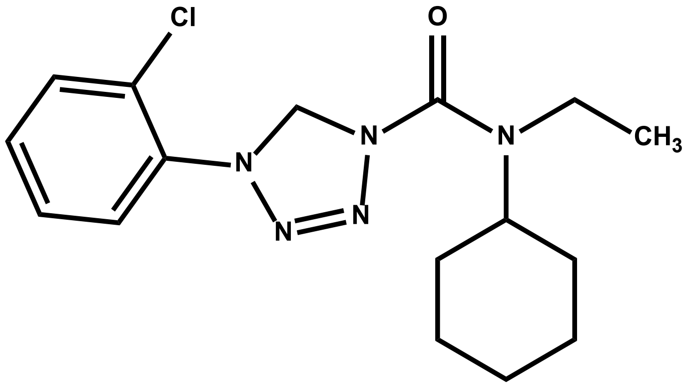
NOMENCLATURE

Common name: fentrazamide
Other name(s): BAY YRC 2388; NBA 061; 4-(2-chlorophenyl)-*N*-cyclohexyl-*N*-ethyl-4,5-dihydro-1*H*-tetrazole-1-carboxamide (IUPAC)
Trade name(s): LECS®; LECSPRO; DOUBLE STAR; INNOVA®; PULSTOP
Chemical family: tetrazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

fentrazamide



Molecular formula: $C_{16}H_{20}ClN_5O_2$
Molecular weight: 349.82 g/mole
Description: Colorless crystals
Density: 1.30 g/mL (20 C)
Melting point: 79 C
Boiling point: Not measurable due to the thermal decomposition
Vapor pressure: 5 x 10^{-7} Pa (20 C)
Stability: Stable
Solubility:
water 2.3 mg/L (20 C)
organic solvents g/L (20 C):
2-propanol 32
xylene >250
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 3.60 (20 C)

HERBICIDAL USE

Fentrazamide is used for the control of barnyardgrass and annual sedges in rice (1). Fentrazamide at 200 to 300 g ai/ha has shown excellent efficacy against barnyardgrass within a wide range of growth stages from PRE up to 3 leaf stage of the weed with good compatibility to rice. Combinations of fentrazamide with sulfonylurea herbicides such as bensulfuron-methyl, cyclosulfamuron and imazosulfuron provide excellent broadleaf weed control that covers the entire weed spectrum of transplanted rice grown in Japan.

USE PRECAUTIONS

Fire hazard: Fentrazamide is non-flammable.
Corrosiveness: Product is non-corrosive.
Storage stability: Technical active ingredient is not sensitive to oxidizing or reducing agents.
Cleaning glassware/spray equipment: Wash equipment and glassware with water ad detergent.
Emergency exposure: If on skin, wash with plenty of soap and water. Get medical attention if irritation persists. If in eyes, flush with plenty of water. Call a physician if irritation persists. If inhaled, remove victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. However, appears to arrest cell division in the root and shoot meristematic regions (1) (more details on page 14)
Symptomology: Susceptible plant species exhibit halted growth and distortion of elongated tissue.
Absorption/translocation: Fentrazamide is absorbed through the roots and shoots of susceptible plants.
Metabolism in plants: NA
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: No resistant weed biotypes are known to this mode of herbicide action.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 400-3400 mL/g in Japanese paddy soil
Transformation:
Photodegradation: Fentrazamide photolyzes rapidly in aquatic systems. The half-life of photodegradation in pure water (25 C) is about 20 d, whereas in natural water (25 C) is 10 d
Other degradation: Fentrazamide is susceptible to chemical hydrolysis. The rate of chemical degradation is dependent on pH. Half-lives of chemical hydrolysis were > 300 d at pH 5 (25 C), > 500 d at pH 7 (25 C), and about 70 d at pH 9 (25 C). Microbial metabolism under paddy conditions also degrades fentrazamide.
Persistence: Fentrazamide dissipates rapidly in natural waters and is readily degraded. The half-life of soil metabolism was about 30 d in volcanic soil and 20 d in alluvial soil.
Mobility: Fentrazamide had low mobility in Japanese paddy soils.
Volatilization: NA
Formulation effects: Environmental fate properties are unaffected by formulation type.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fentrazamide unless otherwise indicated.
Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >5000 mg/L; Primary eye irritation rabbit, non irritating; Skin irritation rabbit, negative; Skin sensitization guinea pig, negative.

Subchronic toxicity: Subchronic studies showed that all species tested tolerate high levels of fentrazamide for prolonged periods of time with few signs of toxicity.

Chronic toxicity: Chronic studies showed that all species tested tolerate high levels of fentrazamide for prolonged periods of time with few signs of toxicity

Teratogenicity:

Rat: Non-teratogenic

Rabbit: Non-teratogenic

Reproduction: NA

Mutagenicity:

Gene mutation: Ames and CYT in vitro mutagenicity tests were negative

Wildlife:

Silkworm NOEC, 100 mg/kg; Honey bee topical LD_{50}, >150 mg/bee; Daphnia 3-h EC_{50}, >10 mg/L; Rainbow trout 48-h LC_{50}, 3.4 mg/L; Carp 48-h LC_{50}, 3.2 mg/L

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: See Yanagi, 2000

Purification of technical: See Yanagi, 2000

Analytical methods: See Yanagi, 2000

Historical: Fentrazamide was discovered by Bayer AG and is under development in Japan AG and Nihon Bayer Agrochem.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Yasui, K. et. Al. 1997. Proc. Brighton Crop Prot. Conf. – Weeds, pp. 67-72.
2. Yanagi, A. 2000. Pflanzenschutz-Nachrichten Bayer. 54:5-12.

flazasulfuron

CAS #: 104040-78-0

2^(B)

N-[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]-3-(trifluoromethyl)-2-pyridinesulfonamide

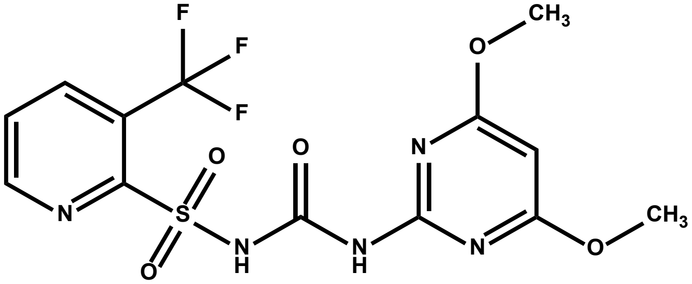
NOMENCLATURE

Common name: flazasulfuron (BSI, draft E-ISO)
Othername(s): SL-160; OK-1166; 1-(4,6-dimethoxypyrimidin-2-yl)-3-(3-trifluoromethyl-2-pyridylsulfonyl)urea (IUPAC)
Trade name(s): KATANA; MISSION®; SHIBAGEN; CHIKARA
Chemical family: pyrimidinylsulfonylurea; sulfonlyurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

flazasulfuron



Molecular formula: $C_{13}H_{12}F_3N_5O_5S$
Molecular weight: 407.3 g/mole
Description: Odorless, white crystalline powder
Density: 1.61 g/mL
Melting point: 147-150 C
Boiling point: NA
Vapor pressure: $<1.3 \times 10^{-5}$ Pa; Henry's Law constant, 2.58 Pa m^3 mol^{-1}
Stability: DT_{50} in water 11 d (25 C)
Solubility:
water, 27 mg/L (pH 5); 2100 mg/L (pH 7); not stable at pH 9
organic solvents (g/L 25 C)

octanol 0.2	methanol 4.2
acetone 22.7	toluene 0.56
acetonitrile 8.7	hexane 0.5 mg/L

pK_a: 4.37 (20 C) (weak acid)
K_{ow}: log K_{ow} = -0.06

HERBICIDAL USE

PRE and POST control of grass and broadleaf weeds and sedges (esp. *Cyperus brevifolious* and *Cyperus rotundus*) in warm season turf (*Zoysia* and *Cynodon spp.*) at 25-100 g/ha. Also used in vines and sugar cane at 35-75 g/ha.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Non-corrosive
Storage stability: NA
Cleaning glassware/spray equipment: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Susceptible plants exhibit chlorosis followed by necrosis of leaf tissue. Newer growth is affected first.
Absorption/translocation: Absorbed by roots and foliage. Primarily translocated by the phloem.
Metabolism in plants: Rearrangement of the sulfonylurea bridge is the primary degradation pathway, followed by hydrolysis and *O*-demethylation reactions. The DT_{50} of flazasulfuron in tolerant turf grasses was < 1 day compared to 9-10 days in sensitive plant species.
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: Weed species resistant to other sulfonylurea herbicides would be expected to be resistant to flazasulfuron.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 30-43 mL/g
Transformation:
Other degradation: Flazasulfuron is rapidly degraded in the soil with a DT_{50} of 13-16 d. Metabolism in soil appears to be via hydrolytic reactions.
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flazasulfuron unless otherwise indicated.
Acute toxicity:
Oral LD_{50} for rats & mice, >5000 mg/kg; Dermal LD_{50} for rats, >2000 mg/kg; Eye irritation rabbit, moderate; Skin irritation rabbit, none; Skin sensitization guinea pigs, none
Chronic toxicity:
24-month dietary, rat: 1.3 mg/kg/d
Mutagenicity:
Gene mutation: Ames test negative
Structural chromosome aberration: Negative
DNA damage/repair: Negative
Wildlife:
Acute oral LD_{50} for Japanese quail, >2000 mg/kg; LC_{50} for carp, >20 mg/L; Daphnia 48-hr LC_{50}, >20 mg/L; LD_{50}, >100 mg/bee
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: First introduced by Ishihara Sangyo Kaisha Ltd in 1989 in Japan, acquired by Zeneca in 1997.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Roberts, T. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.

florasulam

CAS #: 145701-23-1

2$^{(B)}$

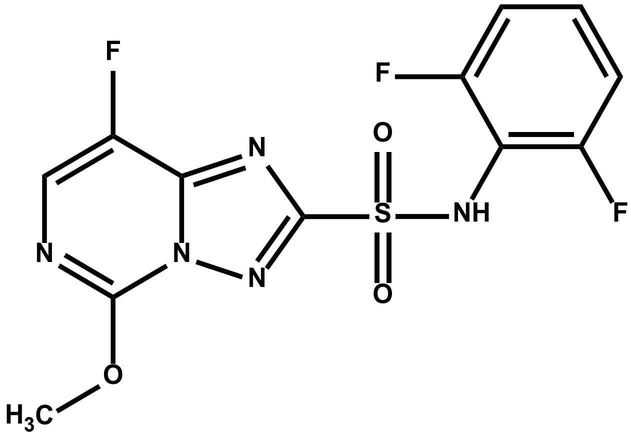
N-(2,6-difluorophenyl)-8-fluoro-5-methoxy(1,2,4) triazolo(1,5-*c*)pyrimidine-2-sulfonamide

NOMENCLATURE

Common name: florasulam
Other name(s): XDE-570; 2',6',8'-trifluoro-5-methoxy[1,2,4] triazolo[1,5-*c*]pyrimidine-2-sulfonanilide (IUPAC)
Trade name(s): DEFENDOR, ORION, PRIMUS®; BOXER®
Chemical family: sulfonanalide; triazolopyrimidine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
florasulam



Molecular formula: $C_{12}H_8F_3N_5O_3S$
Molecular weight: 359.28 g/mole
Description: Off-white; no discernible odor
Density: 1.53 g/mL (22 C)
Melting point: 193.5 to 230.5 C (decomposes)
Vapor pressure: 1.0 x 10^{-5} Pa (25 C)
Solubility:
water, 84 mg/L (pH 5); 6360 mg/L (pH 7); 94,200 mg/L (pH 9); 121 mg/L in distilled water
Other solvents (g/L)
acetone 123
acetonitrile 72.1
dichloromethane 3.75
ethyl acetate 15.9
n-Heptane 0.000019
methanol 9.81
1-octanol 0.184
xylene 0.227
pK$_a$: 4.54 (weak acid)
K$_{ow}$: log K_{ow} =1.00 (pH 4); -1.22 (pH 7); -2.06 (pH 10)

HERBICIDAL USE

Florasulam is a broadleaf herbicide for use in cereals and turf; cereals and turf will be the key North American market. It may be used in winter and spring cereals including wheat, barley, oats, rye and triticale (3-leaf to flag leaf typical application timing in cereals). Florasulam possesses both soil and foliar activity. However, uses will be mainly limited to post emergence due to the extremely short half-life in soil.

Florasulam is highly selective to cereals, but very active on weeds in the plant families Asteraceae, Polygonaceae, Caryophyllaceae, Rubiaceae, and Crucifereae. In the field, efficacy trials have shown excellent activity on these broadleaf weeds in cereal crops - *Galium aparine, Stellaria media, Matricaria* spp*, Polygonum convolvulus, and Papaver rhoeas.* In turf, florasulam has excellent activity on many of these same weeds including *Taraxacum officinale* when applied in the early spring or fall. Florasulam displays herbicidal activity at very low doses, resulting in low environmental impact. Typical global use rates for cereals range from 2.5 to 7.5 g ai/ha and for turf single applications are 15 g ai/ha with up to 3 such applications allowed per season.

USE PRECAUTIONS

Fire hazard: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxyacid synthase (AHAS). (more detail on page 12)
Symptomology: Growth in sensitive species is retarded within a matter of hours of application although visible effects may not be observed for several days. Symptoms appear first in the upper meristematic region of the plant as chlorosis and necrosis. The upper new leaves often take on a wilted appearance. The effects then spread to the remaining parts of the plant. Reddening of the midrib and veins is observed in some species. Complete desiccation of the plant typically occurs in 14-21 d under ideal growing conditions, and up to 6-8 weeks under less than ideal conditions.
Absorption/translocation: Florasulam can be absorbed by roots or foliage of plants and is translocated through both the xylem and phloem to growing points. In tolerant plants, there is less herbicide uptake and translocation out of treated leaves. The rain-free period for florasulam is 4 h.
Metabolism in plants: The selectivity mechanism is based on a more rapid metabolism in the crop compared to target species. Half-life of florasulam is wheat (3.5 h) and *Galium aparine* (48 h).
Resistance: Numerous weed species have been reported to have evolved resistance to ALS-inhibiting herbicides. Resistant biotypes are naturally occurring and are slightly different in genetic make-up. In North America, *Sinapis arvensis*, *Galeopsis tetrahit, Galium spurium, Stellaria media, Kochia scoparia, Salsola kali and Sonchus asper* have documented cases of resistance to ALS inhibitor herbicides. Of these, three species will be important to florasulam:

Galeopsis tetrahit, Galium spurium and *Stellaria media*. The overall weed spectrum in areas where these weeds are present will require tank mix partners for florasulam. Resistance issues are expected to be manageable through selection of tank mix partners.

BEHAVIOR IN SOIL

Sorption: Florasulam has weak adsorptivity to soil. Soil moisture and soil organic matter have the greatest impact on florasulam adsorption.

K_{oc}: 2 to 69 mL/g; average 18 mL/g

Transformation:

Photodegradation: Minor

Other degradation: Microbial metabolism is the primary degradation mechanism in soil; this requires favorable moisture and temperature for degradation to occur.

Persistence: Florasulam is not persistent in soil, thus poses no threat to rotational crops. Dissipation of florasulam occurs primarily through microbial degradation. Laboratory half-life is 4.5 d at 20 C. Field studies in a wide variety of soils have shown the half-life of florasulam in soil to range from 2 to 18 d. Temperature has the greatest influence on half-life.

Mobility: Although florasulam is potentially mobile in soil, the low use rate coupled with a 2-18 d half-life means it is not likely to contaminate groundwater.

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade florasulam unless otherwise indicated.

Acute toxicity:

Oral rat LD_{50}, >5000 mg/kg; Acute dermal rabbit LD_{50}, >2000 mg/kg; Primary dermal irritation rabbit, mild irritation; Primary eye irritation rabbit, mild irritation; Dermal sensitization potential guinea pigs, none

Teratogenicity: Not teratogenic: NOEL 500 mg/kg dw day (both maternal and embryo-foetal); NOEL 250 mg/kg (maternal); NOEL 750 mg/kg embryo-fetal)

Mutagenicity: Negative (Ames test)

Wildlife:

Japanese quail (*Coturnix japonica)* LD_{50}, 1046 mg/kg body weight; LC_{50}, >5000 mg/kg in feed; Bluegill (*Lepomis macrochirus*) 96-h acute LC_{50}, >100 mg/L; Daphnia (*Daphnia magna*) acute EC_{50}, > 292 mg/L, NOEC = 174 mg/L; Rainbow trout (*Oncorhynchus mykiss*) 96-h Acute LC_{50}, >100 mg/L; Atlantic silversides (*Menidia beryllina*) 96-h Acute LC_{50}, >100 mg/L; Grass shrimp (*Palaemonetes pugio*) LC_{50}, >120 mg/L; Eastern oyster (*Crassostrea virginica*) EC_{50}, >125 mg/L; Honey bees (*Apis mellifera*) contact and oral LD_{50}, >100 ug/bee; Earthworms (*Eisenia foetida*) LC_{50}, >1300 mg/kg soil;; Blue green algae (*Anabaena flos-aquae*) EC_{50}, 363 µg/L, 96-h NOEC, 235 µg/L; Freshwater diatom (*Navicula pelliculosa*) EC_{50}, 0.97 mg/L, NOEC, 0.05 mg/L; Marine diatom (*Skeletonema costatum*) EC_{50}, 31.3 mg/L, NOEC, 22.8 mg/L; Duckweed (*Lemna gibba*) 14-d EC_{50}, 1.18 µg/L, NOEC, 0.616 µg/L

SYNTHESIS AND ANALYTICAL METHODS

Analytical methods: The analytical method uses capillary gas chromatography and mass selective detection (GC-MSD)

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

fluazifop-P

(2R)-2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy] propanoic acid

CAS # Acid: 83066-88-0
Butyl ester: 79241-46-6

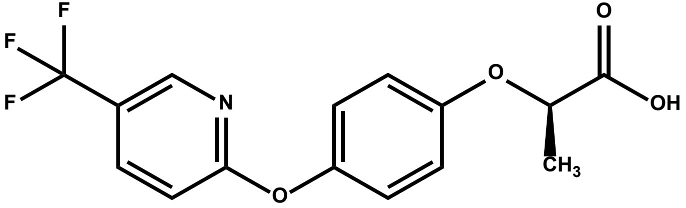
$1^{(A)}$

NOMENCLATURE

Common name: fluazifop-P (ANSI, BSI, ISO, WSSA) for the R isomer; fluazifop (ANSI, BSI, ISO, WSSA) for the racemic mixture of R and S isomers
Other name(s): IH773B; ICIA005; ICIA009; PP009; TF1169; (R)-2-{4-[5-(trifluoromethyl)-2-pyridyloxy] phenoxy} propionic acid (IUPAC); (Butyl ester) fluazifop-P-butyl; butyl (R)-2-{4-[5-(trifluoromethyl)-2-pyridyloxy]phenoxy} propionate (IUPAC)
Trade name(s): FUSILADE®; FUSILADE DX®
Chemical family: aryloxyphenoxy propionate; aryloxyphenoxy propionic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
fluazifop-P acid



Molecular formula: Acid $C_{15}H_{12}F_3NO_4$; Butyl Ester $C_{19}H_{20}F_3NO_4$
Molecular weight: Acid 327.26 g/mole Butyl Ester 383.37 g/mole
Description: Light straw-colored liquid, odorless
Density: 1.22 g/mL (20 C)
Melting point: 5 C for fluazifop-P butyl ester
Boiling point: 164 C (2.67 Pa)
Vapor pressure: 5.4 x 10^{-5} Pa (20 C) for fluazifop-P butyl ester
Stability: Stable to UV light
Solubility:
water 1.1 mg/L (25 C)
organic solvents:
Miscrible in acetone, chloroform, cyclohexanone, dichloromethane, ethyl acetate, n-hexane, methanol, methylene chloride, methylene dichloride, toluene, and xylene.
pK_a: Acid 2.98 (20 C) (weak acid); Butyl Ester None (non-ionizable)
K_{ow}: 1200 (pH 2.6, 20 C); 0.8 (pH 7, 20 C)

HERBICIDAL USE

Fluazifop-P can be applied POST at 0.053-0.21 kg ai/ha in cotton, soybeans, stone fruits, asparagus, carrots, garlic, coffee, endive, pecans, rhubarb, and tabasco peppers. It controls most annual and perennial grass weeds including barnyardgrass, crabgrass spp., downy brome, Panicum spp., foxtail spp., volunteer cereals, shattercane, quackgrass, and johnsongrass. Fluazifop-P has essentially no activity on broadleaf species. An oil adjuvant or non-ionic surfactant is required for maximum efficacy.

USE PRECAUTIONS

Fire hazard: The product Fusillade DX is non-flammable; fluazifop-P technical is non-flammable; flash point is 41.8 C
Corrosiveness: Non-corrosive under normal conditions
Storage stability: Stable for >4 mo at 50 C, >7 mo at 37 C, and >16 mo at 5 and 20 C
Cleaning glassware/spray equipment: Clean sprayers with water plus either a commercial tank cleaner or surfactant
Emergency exposure: Slightly irritates eyes
Incompatibilities: Antagonism of grass control has been observed when fluazifop-P has been mixed with certain broadleaf herbicides; incompatible with strong oxidizing agents

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details of page 12)
Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop 1-3 wk after application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.
Absorption: The butyl ester of fluazifop-P is rapidly absorbed into leaves and is rainfast within about 2 h of application (1). Fluazifop-P butyl ester presumably diffuses readily across the plasmalemma. Once inside the cell, the herbicide is rapidly deesterified to fluazifop-P which dissociates in the relatively alkaline cytoplasm. The dissociated anion is "trapped" inside the cell due to its inability to traverse the plasmalemma, a consequence of its negative charge and low lipophilicity.
If fluazifop-P butyl ester is hydrolyzed outside the cell, the relatively acid environment allows a significant proportion of fluazifop acid to remain in the protonated (undissociated) form which readily diffuses across the plasmalemma and into the cell. Upon entering the alkaline phloem cells, the acid dissociates and is trapped inside. Thus, the fluazifop-P concentrations increase in the symplasm.
Translocation: Fluazifop-P principally translocates in the phloem and accumulates in the meristematic regions of the root and shoot. Translocation is slow, however.
Metabolism in plants: Fluazifop-P butyl is hydrolyzed rapidly in plants to the phytotoxic fluazifop-P acid. Quackgrass (fluazifop susceptible) retained 46-79% of applied fluazifop as the acid after 48 h, whereas a small fraction was metabolized to polar and nonpolar conjugates (3).
Non-herbicidal biological properties: Sublethal rates may suppress seed head development in some grass species, such as red rice and downy brome (6,7). At very low rates, 0.014 kg ai/ha fluazifop-P retards grass growth. Activity as a

sugarcane ripener also has been reported.

Mechanism of resistance in weeds: Most fluazifop-P resistance biotypes appear to have an ACCase that is insensitive to the herbicide. However, in diclofop-resistant rigid ryegrass from Australian, cross-resistance to a number of herbicides including fluazifop is not due to reduced ACCase sensitivity (5). Rather resistance may be due to increased herbicide metabolism or by sequestration away from the site of action.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 5700 mL/g for the butyl ester (8).

Transformation:

Photodegradation: Negligible losses

Other degradation: Fluazifop-P butyl ester is rapidly (half-life of <1 wk) deesterified in moist soils to the acid which has a half life of ~3 wk under moist conditions in most soils.

Persistence: Average field half-life of the parent acid is 15 d (8). Fluazifop-P occasionally controls or suppresses grass weeds germinating after application. Degree of residual activity varies with soil characteristics and rainfall. Susceptible rotational crops can be planted 60 d after fluazifop-P application.

Mobility: Fluazifop-P butyl ester has low mobility in soil, while fluazifop-P acid is somewhat more mobile. Neither chemical presents an appreciable risk of groundwater contamination.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fluazifop-P butyl ester unless otherwise indicated.

Acute toxicity:

Fluazifop-P butyl ester technical: Oral LD_{50} male rat, 4096 mg/kg, female rat 2721 mg/kg; Dermal LD_{50} rabbit, >2420 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, slight; Skin sensitization, Guinea pig, no; Eye irritation, rabbit, mild

FUSILADE DX: Oral LD_{50} male rat, >5000 mg/kg, female rat, 5690 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation Male rat, >0.54 mg/L, female rat, >0.77 mg/L; LC_{50}, NA; Skin irritation, rabbit, moderate; Skin sensitization, Guinea pig, no; Eye irritation, rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL 10/mg/kg/d

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail 5-d dietary LD_{50}, >4659 mg/L; Mallard duck oral LD_{50}, >3528 mg/L; 5-d dietary LC_{50}, >4321 mg/L; Honey bee oral LD_{50}, >100; µg/bee topical LD_{50}, >240 µg/bee; Daphnia 48-h LC_{50}, >10 mg/L; Bluegill sunfish 96-h LC_{50}, 0.53 mg/L; Rainbow trout 96-h LC_{50}, 1.37 mg/L

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Several methods can be used, including reaction of 4-(5-trifluoromethyl-2-pyridyloxy)-phenol with butyl 2-chloropropionate and base.

Purification of technical: NA

Analytical Methods: GLC methods are used for analysis of the technical, derivatives, and formulated products. Residue methods are available for certain crops (see AOAC Methods, 1984, 6.353-6.357; CIPAC Handbook, 1988, ID, 106).

Historical: Discovered by Ishihara Sangyo Kaishi, Ltd., and developed jointly with ICI Plant Protection Division (now Syngenta). Great Britain patent 1,599,121 was awarded to Ishihara. Fluazifop-P was first tested for herbicidal activity by ICI Americas in the U.S. in 1981.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Bryson, C. T. 1988. Weed Technol. 2:153.
2. Coupland, D. 1985 Proc. Brit. Crop Prot. Conf.-Weeds, p. 317.
3. Powles, S. B. et al. 1990. Pages 394-406 in M. B. Green , H. M. LeBaron, and W. K. Moberg, eds., Managing Resistance to Agrochemicals. Am. Chem. Soc. Symp. Ser. 421, Washington DC.
4. Richardson, J. M. et al. 1987. Weed Sci. 35:277.
5. Salzman, F. P. et al. 1988. Weed Sci. 35:277.
6. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

flucarbazone-sodium

CAS #: 181274-17-9 $2^{(B)}$

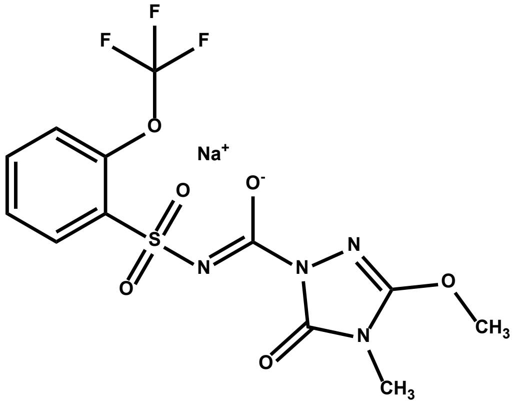
sodium 4,5-dihydro-3-methoxy-4-methyl-5-oxo-*N*-[[2-(trifluoromethoxyphenylsulfonyl)-1*H*-1,2,4-triazole-1-carboxamide

NOMENCLATURE

Common name: flucarbazone-sodium (ISO 1750 accepted)
Other name(s): SJO 0498; BAY MKH 6562; sodium 4,5-dihydro-3-methoxy-4-methyl-5-oxo-*N*-{[2-(trifluoromethoxy)phenyl]sulfonyl}-1*H*-1,2,4-triazole-1-carboximidate (IUPAC)
Trade name(s): EVEREST®; FINESSE® GRASS & BROADLEAF; FINESSE® GRASS & BROADLEAF (MP); VOLCANO
Chemical family: sulfonylaminocarbonyltriazolinone; triazolone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
flucarbazone-sodium



Molecular formula: $C_{12}H_{10}F_3N_4NaO_6S$
Molecular weight: 418.28 g/mole
Description: Colorless and odorless crystalline powder
Density: 1.59 g/mL
Melting point: 200 C
Vapor pressure: 1.32×10^{-7} Pa (20 C)
Solubility: 44 g/L (pH 4-9, 20 C)
pK_a: 1.9 (weak acid)
K_{ow}: log K_{ow} = -0.89 (pH 4); -1.85 (pH 7); -1.89 (pH 9)

HERBICIDAL USE

Flucarbazone-sodium provides activity against grass weeds and several important broadleaf weeds when applied POST to wheat. It has demonstrated activity against wild oat (*Avena fatua*) and green foxtail (*Setaria viridis*). Suggested use rate will be 30 g ai/ha.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: Stable under normal storage conditions.
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Weeds cease to grow and compete with crop soon after application. Further symptoms will develop over 1-4 weeks depending on environmental conditions and include stunting, discoloration and necrosis.
Absorption/translocation: Flucarbazone is absorbed through the foliage and root system. Acropetal and basipetal translocation occurs in treated plants.
Metabolism in plants: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
- **Photodegradation***:* Flucarbazone has a photolytic half-life of >500 d
- **Other degradation**: The primary route of degradation is believed to be microbial

Persistence:
- **Field experiments:** $t_{1/2}$ = 17 d

Volatilization: Minimal

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flucarbazone-sodium unless otherwise indicated.

Acute toxicity:
- Oral LD_{50} rats, >5000 mg/kg; Dermal LD_{50} rats, >5000 mg/kg; Dermal inhalation LC_{50}, Non-irritating

Chronic toxicity:
In chronic studies, no evidence for neurotoxin, genotoxic, carcinogenic potential nor teratogenic or reproductive toxicity

Wildlife:
- **Birds:** Bobwhite quail acute Oral LD_{50}, >2000 mg/kg; subacute dietary LC_{50}, >5000 mg/kg; Mallard duck reproductive NOEC, >223 mg/kg
- **Aquatic organisms:** Bluegill sunfish LC_{50}, >99.3 mg/L; Rainbow trout, >96.7 mg/L; Daphnia, >109 mg/L; Selenastrum capricornutum, 6.4 mg/L; Lemna gibba, 0.0126 mg/L
- **Others:** Earthworm LC_{50}, >1000 mg/kg; Honeybee, non-toxic

Use classification: EPA Category IV

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1. Santel, H.J., B.A. Bowden, V.M. Sorenson, K.H. Mueller. 1999. Proc. 1999 Br. Crop Prot. Conf. Vol. 1:23-28.

flucetosulfuron

CAS #:: 412928-75-7 **$2^{(B)}$**

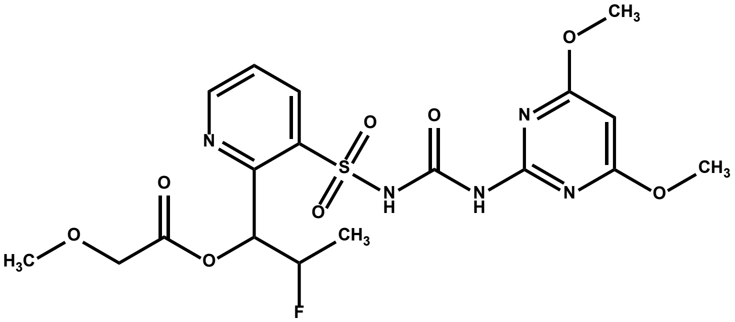
1-[3-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino] sulfonyl]-2-pyridinyl]-2-fluoropropyl methoxyacetate

NOMENCLATURE

Common name: flucetosulfuron (ISO approved in 2003)
Other name(s): LGC-42153; (1*RS*,2*RS*,1*RS*,2*SR*)-1-{3-[(4,6-dimethoxypyrimidin-2-ylcarbamoyl) sulfamoyl]-2-pyridyl}-2-fluoropropyl methoxyacetate (IUPAC)
Trade name(s): NA
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
flucetosulfuron



Molecular formula: $C_{18}H_{22}FN_5O_8S$
Molecular weight: 487.46 g/mole
Description: Odorless, solid white powder (25 C)
Density: NA
Melting point: 178-182 C (decomposition)
Boiling point: NA
Vapor pressure: <1.86 x 10^{-5} Pa (25 C)
Stability: Stable at 50 C for 6 mo; relatively stable at pH 7; unstable in acidic or alkaline media.
Solubility:
water 114 mg/L (25 C)
pK_a: 3.5 (weak acid)
K_{ow}: log K_{ow} = 1.05 (unstated pH)

HERBICIDAL USE

Flucetosulfuron applied to soil or foliage provides broad-spectrum weed control including annual broadleaf weeds, sedges, some grasses such as *Echinochloa* spp. and perennial weeds from 10-40 g ai/ha. Flucetosulfuron applied to foliage provides excellent levels of weed control, mainly broadleaf weeds including *Galium aparine*, *Matricaria* spp. *Papaver rhoeas* at less than 30 g ai/ha in cereal crops, especially wheat and barley.

USE PRECAUTIONS

Fire hazard: Formulated product is non-flammable.
Corrosiveness: Non-corrosive
Storage stability: Keep container tightly closed in a cool, dry place.
Cleaning glassware/spray equipment: NA

Emergency exposure: On ingestion, to not induce vomiting. Dilute swallowed product with large amounts of water. On eye contact, flush with water for at least 15 min. On skin contact, flush with water for at least 15 min. On inhalation, move victim to fresh air.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12).
Symptomology: Growth of treated plants is inhibited within a few h after application, but injury symptoms usually appear 1-2 wk later. Meristematic areas gradually become chlorotic and necrotic, followed by a general foliar chlorosis and necrosis.
Absorption/translocation: Rapid foliar and root absorption. Flucetosulfuron translocates readily in the xylem following root absorption, but less so in the phloem after foliar applications. It accumulates in meristematic areas.
Metabolism in plants: The selectivity mechanism is assumed to be due to metabolism as more rapid recovery of ALS activity was observed in rice as compared to *Echinochloa crus-galli*.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: NA
Other degradation: In aerobic soil degradation studies, the major degradation products of flucetosulfuron resulted from cleavage of the sulfonylurea bridge. In anaerobic soils, the major metabolic reaction was cleavage of the carboxyl ester bond which undergoes hydrolysis of the sulfonylurea bridge.
Persistence: In laboratory studies, aerobic soil metabolism studies indicated that the half-life of flucetosulfuron was 9 d. In anaerobic soils, the half-life is 3 d.
Field experiments: NA
Mobility: NA
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical-grade flucetosulfuron material unless otherwise indicated.**Acute toxicity:** >5000 mg/kg for rats and mice; >2000 mg/kg for dogs
Subchronic toxicity: NA
Chronic toxicity: NA

Teratogenicity: NOEL (13 wks) 200 mg/kg for rats; not oncogenic or teratogenic in rats or mice
Reproduction: NA
Mutagenicity: NA
Wildlife:
Carp (48 h) LC_{50}, >10 mg/kg; Daphnia magna LC_{50} (3 h), >10 mg/kg
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: Discovered by LG Life Sciences. Not sold in the United States and Canada.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): LG Life Sciences
Reference(s):

1, Kim, D. S., S.J. Koo, J. N. Lee, K. H. Hwang, T. Y. Kim, K. G. Kang, K. S. Hwang, G. H. Joe, J. H. Cho and D. W. Kim. 2003. Flucetosulfuron: a new sulfonylurea herbicide. Proceedings of the BCPC International Congress – Crop Science & technology 2003, Vol. 1, 87-92.
2. Kim, K., K. H. Liu, S. H. Kang, S. J. Koo, and J. H. Kim. 2003. Degradation of the sulfonylurea herbicide LGC-42153 in flooded soil. Pest Manag. Sci. 59:1037-1042.
3. Kim, J., K. H. Liu, S. H. Kang, S. J. Koo, and J. H. Kim. 2003. Aerobic soil metabolism of a new herbicide, LGC-42153. J. Agri. Food Chem. 51:710-714.

flufenacet

CAS #: 142459-58-3

15$^{(K_3)}$

N-(4-fluorophenyl)-N-(1-methylethyl)-2-[[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]oxy]acetamide

NOMENCLATURE

Common name: flufenacet (ISO approve

Other names: fluthamide; thiafluamide; thiadiazolamide; BAY FOE 5043; 4'-fluoro-*N*-isopropyl-2-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yloxy]acetanilide (IUPAC)

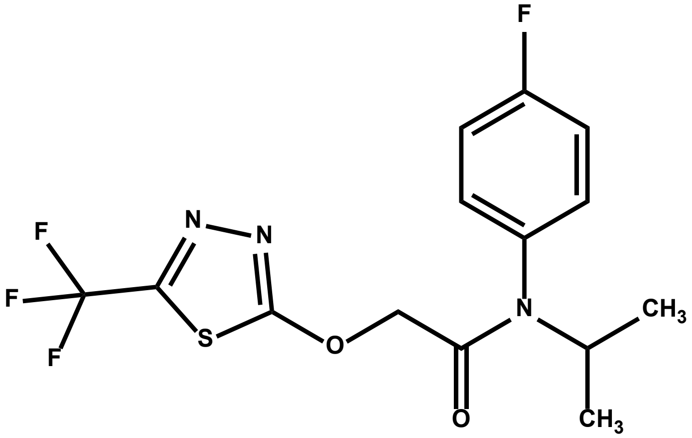
Trade name(s): AXIOM™ DF; DEFINE™ DF; DEFINE™ SC; DOMAIN™ DF; EPIC® DF; RADIUS™

Chemical family: acetamide; anilide; oxyacetamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

flufenacet



Molecular formula: $C_{14}H_{13}F_4N_3O_2S$

Molecular weight: 363.33 g/mole

Description: White solid

Density: 1.31 g/mL

Melting point: 75.5-77 C

Boiling point: Decomposes

Vapor pressure: 2 x 10^{-5} Pa (20 C)

Stability: Not thermally stable

Solubility:

water 56 mg/L (25 C)
organic solvents g/L (20 C):
n-hexane 8.7 toluene 200
2-propanol 170 1-octanol 88
dichloromethane >200
polyethylene glycol 74
polyethylene glycol + ethanol 160
acetone >200 dimethyformamide >200
acetonitrile >200 dimethysulfoxide >200

pK_a: None (non-ionizable)

K_{ow}: 1600 (24 C); log K_{ow} = 3.20

HERBICIDAL USE

Flufenacet may be applied either preplant surface, PPI and/or PRE and is selective in a variety of crops including corn, soybeans, cotton, peanut, wheat, sunflower, and potatoes (1). Presently, it is being registered only as a premixture with a low rate of metribuzin (4:1 ratio) for the corn and soybean markets under the trade name AXIOM™. Use rates of AXIOM range from 0.6 to 1.1q kg/ha. Flufenacet controls most annual grasses and certain small-seeded broadleaf weeds and suppresses nutsedge. The AXIOM premixture improves the small-seeded broadleaf control as compared to flufenacet alone.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: Flufenacet and AXIOM are non-corrosive to equipment and metal surfaces.

Storage stability: Shelf-life of AXIOM is at least one year at moderate temperature and below. At temperatures of 40 C and above, there is a loss of active ingredient. Store in a cool dry place. Avoid storage at 49 C. The maximum 30-day average storage temperature should not exceed 38 C.

Cleaning glassware/spray equipment: Clean sprayers with water and detergent; clean pump, nozzles and screens separately.

Emergency exposure: Flush eyes with water for at least 15 minutes. Wash skin with soap and water. If flufenacet or AXIOM are ingested, induce vomiting.

Incompatibilities: Flufenacet and AXIOM are compatible with most other pesticides, can be applied in liquid fertilizers and may be impregnated on dry fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. However, appears to arrest cell division in the root and shoot meristematic regions (1) (more details on page 14)

Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Susceptible grasses that emerge appear twisted and malformed with leaves which are tightly rolled in the whorl and are unable to unroll naturally. Leaves do not emerge properly from the coleoptile.

Absorption/translocation: Flufenacet is taken up by the roots and emerging shoots (coleoptiles) of treated plants. It translocates mainly in the xylem, moving into the stems and leaves of treated plants. Foliar application of flufenacet to grass weeds revealed very little basipetal translocation of the active ingredient to the shoot and root (1).

Metabolism in plants: Flufenacet is metabolized rapidly in tolerant crops such as corn, soybeans and sorghum (2). No parent compound is found in these plants following a preemergence application of flufenacet to the soil. Although a number of metabolites have been isolated, conjugation with glutathione is the first major step in the degradation pathway of this herbicide in tolerant plants. Glutathione *S*-transferases (GSTs) which catalyze the conjugation of flufenacet with glutathione have been isolated (2). GST activity using flufenacet as substrate was 3 to 4 times higher in corn seedlings that other crop and weed species (2). Other metabolites of flufenacet found in plants include hydrolytic and oxidative products of the parent herbicide.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Flufenacet is adsorbed moderately to soil. Adsorption is greater to soils with high clay and OM content.

K_{oc}: K_{oc} 613 mL/g and K_d 1.0 mL/g for sand with 0-.3% OM, 3% clay, and pH 5.0; K_{oc} 742 mL/g and K_d 1.6 mL/g for sandy loam with 0.4% OM, 7.5% clay and pH 6.4; K_{oc} 354 mL/g and K_d 4.8 mL/g for sandy loam with 2.4% OM, 5% clay, and pH 6.4; K_{oc} 213 mL/g and K_d 3.2 mL/g for silt loam with 2.9% OM, 17% clay and pH 5.9; K_{oc} 233 mL/g and K_d 2.7 mL/g for clay loam with 2.2% OM and 29% clay and pH 6.4; K_{oc} 113 mL/g and K_d 4.9 mL/g for loam with 7.3% OM, 8% clay, and pH 7.1; K_{oc} 144 mL/g and K_d 4.0 mL/g for silt loam with 4.7% OM, 24% clay and pH 7.3.

Transformation:

Photodegradation: Photodecomposition is insignificant under field conditions; half-life >30 days in sterile water at pH 5.0 and 25 C using artificial sunlight. Half-life >30 days on a sandy loam surface at 6.2 ppm and 25 C using artificial sunlight.

Other degradation: Microbial degradation is the principal means of dissipation in soil. Half lives for aerobic microbial degradation range from 10 to 34 days in various soils at approximately 1.0 ppm at 20-21 C. Major degradation products under aerobic conditions are *N*-(4-fluorophenyl)-2-hydroxy-*N*(1-methylethyl)acetamide, 4-fluoro-*N*-methylaniline-sulfoacetamide, [4-fluorophenyl) (1-methylethyl) amino] oxoacetic acid, and 3-trifluoromethyl-1,3,4-thiadiazol-2(3H)-one. Flufenacet is metabolized slowly under anaerobic conditions with a half-life of 240 d at 1.0 mg/kg and 21 C. Non-biological degradation is negligible.

Persistence: Short to moderate persistence

Field experiments: Half-life was 29 d at 0.1 cm for a dissipation study in Wisconsin on loamy sand with 0.9% Om and pH 5.7. Half-life was 62 d at 0-15 cm for a dissipation study in North Carolina on loamy sand with 0.5% OM and pH 5.6.

Mobility: Laboratory studies indicate that FLUFENACET has low to moderate mobility in most soil textures. In field experiments conducted in Wisconsin and North Carolina, no residues of Flufenacet and four metabolites (LOD 10 mg/L) have been detected below 46 cm.

Volatilization: NA. Studies not conducted due to low vapor pressure of flufenacet.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flufenacet unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1617 mg/kg, female rat, 589 mg/ Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, >3740 mg/L; Primary eye irritation rabbit, negative; Skin irritation rabbit, negative; Skin Sensitization guinea pig, negative

Flufenacet WG 60 formulation: Oral LD_{50} male rat, 1365 mg/kg, female rat 371 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50} rat, >5230 mg/L; Primary Eye irritation rabbit, mild; Skin irritation rabbit, negative; Skin sensitization guinea pig, positive

AXIOM DF formulation: Oral LD_{50} male rat, 2347 mg/kg, female rat, 2072 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50} rat, >977 mg/L; Primary eye irritation rabbit, mild; Skin irritation rabbit, negative; Skin sensitization guinea pig, negative

Subchronic toxicity:

90-d dietary mouse: Generally characterized as involving structural and/or functional alterations in liver-, hematologic/spleen-, and thyroid-related endpoints

90-d dietary rat: NOEL; no adverse effects at up to 25 mg/kg in males (1.7 mg/kg/d) and 100 mg/kg females (7.2 mg/kg/d); generally characterized as involving structural and or functional alterations in liver-, kidney-, hematologic/spleen-, and thyroid-related endpoints

90-d dietary dog: NOEL; no adverse effects at up to 50 mg/kg (1.67 and 1.70 mg ai/kg/d for males and females, respectively); generally characterized as involving structural and/or functional alterations in liver-, kidney-, hematologic/spleen, and thyroid-related endpoints

Chronic toxicity:

18-mo dietary, mouse: Oncogenicity: negative (no evidence)

24-mo dietary, rat: NOEL; No adverse effects at up to 25 mg/kg (1.2 and 1.5 mg ai/kg/d for males and females, respectively); generally characterized as involving structural and/or functional alterations in liver-, kidney-, hematologic/spleen-, and thyroid-related endpoints

12-mo dietary, dog: NOEL; No adverse effects at up to 40 mg/kg (1.29 and 1.14 mg ai/kg/d for males and females, respectively); generally characterized as involving structural and/or functional alterations in liver-, kidney-, hematologic/spleen-, and thyroid-related endpoints

Teratogenicity:

Rat: NOEL maternal and developmental 25 mg/kg/d; decreased maternal body weight and food consumption, reduced fetal weight, increased, increased delayed ossification, and/or increased variation in some skeletal elements; not teratogenic

Rabbit: NOEL maternal 5 mg/kg/d, developmental 25 mg/kg/d; decreased maternal body weight, histoparhological changes in maternal liver, decreased fetal weight, increased delayed ossification, increased skeletal variations; not teratogenic

Reproduction:

Rat: NOEL reproductive 500 mg/kg, maternal 20 mg/kg decreased maternal body weight, increased maternal liver weight, histopathological changes in maternal liver; not a reproductive toxin

Mutagenicity: Not mutagenic in various tests

Wildlife: Bobwhite quail oral LD_{50}, 1608 mg/kg; 8-d dietary LC_{50}, >5317 mg/kg; Mallard duck 8-d dietary LC_{50}, >4970 mg/kg; Earthworm acute LC_{50}, 226 mg/kg; Honey bee LD_{50}, >225 mg/bee; Daphnia 48-h EC_{50}, 39.4 mg/L; Bluegill sunfish 96-h LC_{50}, 2.4 mg/L; Rainbow trout 96-h LC_{50}, 3.5 mg/L; Sheepshead minnow 96-h LC_{50}, 3.31 mg/L; Eastern oyster 96-h EC_{50}, 12.6 mg/L; Shrimp 96-h LC_{50}, 2.83 mg/L

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Flufenacet is obtained be reacting equivalent quantities of 2-methylsulfonyl-5-trifluoromethyl-1,3,4-thiadiazole with 2-hydroxy-[*N*(4-fluorophen-yl)-*N*-isopropyl] acetamide in the presence of sodium hydroxide in acetone at 0 to 5 C (1).

Purification of technical: NA**Analytical methods:** An analytical method for measuring the residues of flufenacet and its metabolites in crop matrices has been developed (3). Crop residues were briefly oxidized and hydrolyzed by fluoroaniline by digesting the crop mixture with sulfuric acid. The fluoroaniline was separated from the crop matrix by steam distillation after making the crop digest basic. The fluoroaniline was extracted from the s and derivatized. The derivative was measured by gas chromatography/mass spectrpscopy-selected ion monitoring (GC-MS-SIM) (3).

Historical: Flufenacet was initially synthesized by Bayer AG in 1988 and its herbicidal properties described shortly thereafter (1). The product was introduced at the 1994 meeting of the North Central Weed Control Conference. In 1996, EPA approved Experimental Use Permits (EUP) for the use of AXIOM in corn and soybeans grown in six mid-western states.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Pflanzenschutz-Nachrichten Bayer. 1997. Special Issue on FLUFENACET, 50(2): 101-194.
2. Bieseler B. et al. 1997. Pflanzenschutz-Nachrichten, Bayer 50:117.
3. Gould, T.J. et al. 1997. Pflanzenschutz-Nachrichten, Bayer 50:199.

flufenpyr-ethyl

CAS #: 188489-07-8

14$^{(E)}$

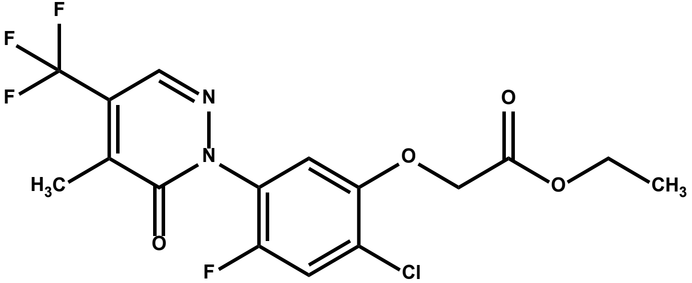
ethyl [2-chloro-4-fluoro-5-[5-methyl-6-oxo-4-(trifluoromethyl)-1(6H)-pyridazinyl]phenoxy]acetate

NOMENCLATURE

Common name: flufenpyr-ethyl (ISO 1750 provisional)
Other name(s): V-3153; S-3153; ethyl 2-chloro-5-[1,6-dihydro-5-methyl-6-oxo-4-trifluoromethyl)pyridazin-1-yl]-4-fluorophenoxyacetate (IUPAC)
Chemical family: phenylpyrazole; pyridazinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
flufenpyr-ethyl



Molecular formula: $C_{16}H_{13}ClF_4N_2O_4$
Molecular weight: 408.7 g/mole
Description: Off-white powder
Density: 0.155 g/mL
Boiling point: NA
Vapor pressure: 6.80 x 10^{-5} Pa
Stability: stable at ambient temperatures
Solubility: water, 2.3 mg/L (20 C); soluble in most organic solvents
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 3.49

HERBICIDAL USE

Flufenpyr-ethyl is being developed for postmergence broadleaf weed control in soybean.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable at ambient temperatures
Emergency exposure: Ingestion: Drink 1-2 glasses of water or milk and induce vomiting by touching the back of the throat with finger. Do not induce vomiting. Eyes: Flush eyes immediately with plenty of water while holding eyelids open.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Sensitive plants display symptoms within hours of application. Symptoms include contact type of necrosis and bronzing.

leaves and roots; limited translocation. Leaf absorption can be increased by adding a surfactant.
Metabolism in plants: NA
Mechanism of resistance in weeds: None reported.

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Photodegradation: NA
Other degradation: NA
Persistence: NA
Mobility: NA
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Acute toxicity:
Oral LD_{50} rats, > 5000 mg/kg; Dermal $LD_{50,}$ > 5000 mg/kg; Inhalation $LC_{50,}$ 5 mg/L air
Subchronic toxicity:
No signs of toxicity were observed in rats exposed by dermal route to 1000 mg/kg/d technical. Slight histological changes in the liver and kidney were observed in rats treated with 6000 mg/kg or greater. NOEL (rats) 300 mg/kg/d; (dogs) 1000 mg/kg/d.
Chronic toxicity: NOEL (dogs) 1000 mg/kg/d
Teratogenicity: Non-teratogenic
Reproduction: No reproductive or neonatal toxicity was observed in a two generation rat reproduction study
Mutagenicity: Negative in Ames assay
Wildlife:
Avian toxicity: Oral LD_{50} bobwhite quail, > 2250 mg/kg; Dietary $LC_{50,}$ > 5620 mg/kg
Aquatic toxicity: LC_{50} bluegill sunfish, 2.7 mg/L (96 h); LC_{50} rainbow trout, 3.7 mg/L (96 h); EC_{50} Daphnia magna, > 3 mg/L (48 h); Oral $LD_{50,}$ > 25 ∝g/bee
Use classification: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Valent

flumetsulam

CAS #: 98967-40-9 **$2^{(B)}$**

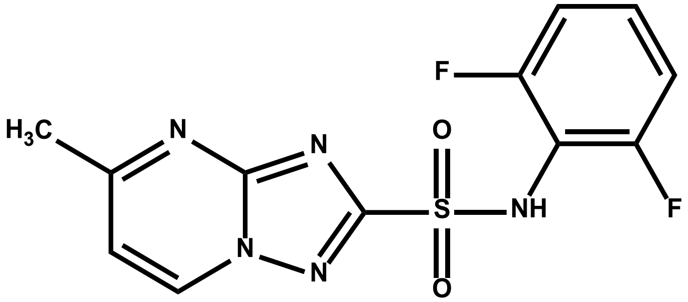
N-(2,6-difluorophenyl)-5-methyl[1,2,4]triazolo[1,5-*a*]
pyrimidine-2-sulfonamide

NOMENCLATURE

Common name: flumetsulam (ANSI, ISO, WSSA).
Other name(s): DE-498; XDE-498; 2',6'-difluoro-5-methyl[1,2,4]triazolo[1,5-a]pyrimidine-2-sulfonanilide (IUPAC)
Trade name(s): ACCENT® GOLD WDG; FRONTROW; HORNET WDG, PYTHON WDG
Chemical family: sulfonanilide; triazolopyrimidine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
fluemetsulam



Molecular formula: $C_{12}H_9F_2N_5O_2S$
Molecular weight: 325.29 g/mole
Description: Off-white to light tan solid
Density: 1.77 g/mL
Melting point: 253 C
Boiling point: NA
Vapor pressure: 3.7×10^{-4} Pa (25 C)
Stability: Stable to sunlight
Solubility:
- water, 49 mg/L (pH 2.5, 25 C); 5600 mg/L (pH 7, 25 C)
- organic solvents g/100 mL (25 C):
  - acetone <1.6
  - methanol <0.4
  - *n*-hexane insoluble
  - xylene insoluble

pK_a: 4.6 (weak acid)
K_{ow}: 6.2×10^{-2} (pH 3.4, 25 C)

HERBICIDAL USE

Flumetsulam containing products are labeled both for soil and POST applications in corn and soybean. Soil applications offer great flexibility in that treatments can be made pre-plant, pre-emergence, or pre-plant incorporated in various tillage systems. Flumetsulam as a soil herbicide controls many key broadleaf weeds such as wild mustard, pigweed spp., kochia, lambsquarters, wild buckwheat, nightshade spp., and velvetleaf. The molecule has little activity against grasses. Copacks and mixes of flumetsulam products are also labeled for POST use in both corn and soybean; these include HORNET (for POST use in corn) and FRONTROW (a POST soybean co-pack).

USE PRECAUTIONS

Fire hazard: PYTHON WDG and HORNET WDG are dry and non-combustible.
Corrosiveness: Flumetsulam is non-corrosive. Flumetsulam does not react with stainless or mild steel at 50 C.
Storage stability: PYTHON WDG and HORNET WDG have no temperature restrictions.
Cleaning glassware/spray equipment: Clean equipment with water.
Emergency exposure: Wash skin with soap and water. If flumetsulam products are ingested, do not induce vomiting; call a physician or poison control center. If available, administer 6-8 heaping teaspoons activated charcoal with a large quantity of water.
Incompatibilities: None known; compatible with most dry or liquid fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Most sensitive weed species are killed before emergence, but weeds may die after emergence under some conditions. Emerged sensitive species exhibit stunting, interveinal chlorosis, veinal discoloration (purpling), and necrosis within 1-3 wk.
Absorption/translocation: Primarily absorbed by roots, with some absorption by emerging shoots. Flumetsulam is readily translocated from roots to shoots and from shoots to roots.
Metabolism in plants: Half-life is 2 h in tolerant corn, 18 h in tolerant soybeans, and 104 h in susceptible redroot pigweed. No metabolism was observed after 144 h in highly susceptible velvetleaf.
Non-herbicidal biological properties: None Known.
Mechanism of resistance in weeds: Numerous weed species (including prickly lettuce, kochia, Russian thistle, cocklebur, ragweed, and pigweeds and others) have been reported to have resistance to ALS-inhibiting herbicides. Resistant biotypes are naturally occurring and are slightly different in genetics. In addition, cross-resistance can occur to different classes of ALS-inhibitors. If ALS-resistant biotypes are present, application of an AS-inhibiting herbicide typically will not control these weeds.

BEHAVIOR IN SOIL

Sorption: Adsorbed much more tightly to organic matter than to clay; greater adsorption at lower vs. higher soil pH
- **K_{oc}:** Average 15 L/kg
- **K_d:** Range 0.1 to 1 L/kg

Transformation:
Photodegradation*:* Soil photolysis is not a major route

of flumetsulam degradation.

Other degradation:

The first order half-life was strongly related to adsorption K_d in that flumetsulam degraded more quickly in soils which adsorbed it less strongly. Adsorption of flumetsulam, in turn, decreased on higher pH soils, but increased with higher organic carbon content. Half-lives were thus influenced by both pH and soil organic carbon: These results mean that persistence of flumetsulam in the field should be shorter for soils with higher pH, but longer for soils with higher organic carbon contents.

Persistence: Laboratory half-lives in 23 soils ranged from 2 weeks to 4 months; 80% of the soils had a half-life of 2 months.Residues from flumetsulam do not injure soybeans, corn, alfalfa, drybeans, peas, peanuts, potatoes, small grains, rice, grain sorghum, and tobacco planted 1 yr after application.

Mobility: NA

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flumetsulam unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 1.2 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none.

Subchronic toxicity:

90-d dietary, mouse: NOEL 1000 mg/kg/d
90-d dietary, rat: NOEL 250 mg/kg/d
90-d dietary, dog: NOAEL <500 mg/kg/d

Chronic toxicity:

18-m dietary, mouse: NOEL >1000 mg/kg/d; not oncogenic
24-m dietary, rat: NOAEL 500 mg/kg/d (male), 1000 mg/kg/d (female); not oncogenic
12-m dietary dog: NOAEL 100 mg/kg/d

Teratogenicty:

Rat: NOEL >1000 mg/kg/d; not teratogenic
Rabbit*:* NOEL 700 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 1000 mg/kg/d; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative
DNA damage/repair: Rat UDS, negative
in vivo mouse micronucleus, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50} >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Honey bee contact LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >250 mg/L; Bluegill sunfish 96-h LC_{50}, >300 mg/L; Fathead minnow 96-h LC_{50}, >293 mg/L; Oyster EC_{50}, >173 mg/L; Rainbow trout 96-h LC_{50}, >300 mg/L; Silverside minnow 96-h LC_{50}, 380 mg/L; Grass shrimp 96-h LC_{50}, >349 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: Discovered in 1984. EUP trials were conducted in 1992 and 1993. First registered Oct. 20, 1993 as BROADSTRIKE + TREFLAN.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences; DuPont Crop Protection

flumiclorac

[2-chloro-4-fluoro-5-(1,3,4,5,6,7-hexahydro-1,3-dioxo-2*H*-isoindol-2-yl)phenoxy]acetic acid

CAS # Acid: 87547-04-4
Pentyl ester: 87546-18-7

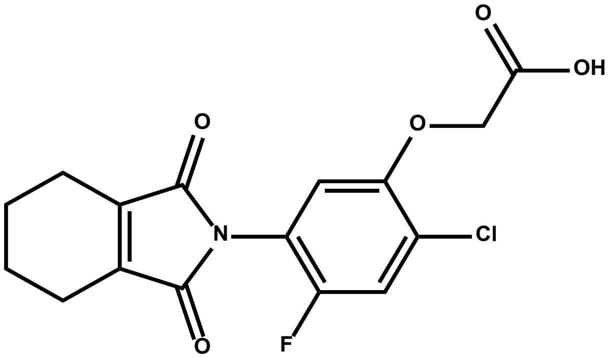
14$^{(E)}$

NOMENCLATURE

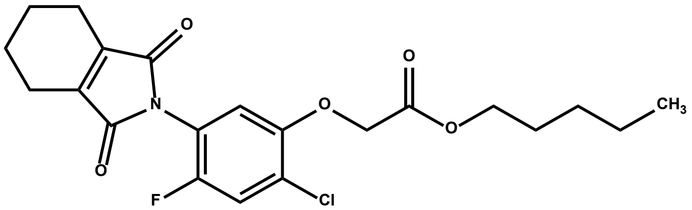
Common name: flumiclorac (ANSI, ISO, WSSA)
Other name(s): S-2303; V-23031; flumiclorac-pentyl (ISO); *Acid* [2-chloro-5-(cyclohex-1-ene-1,2-dicarboximido)-4-fluororophenoxy]acetic acid (IUPAC); *Pentyl ester* pentyl 2-chloro-4-fluoro-5-(3,4,5,6-tetrahydrophthalimido) phenoxyacetate (IUPAC)
Trade name(s): RESOURCE®; SUMIVERDE®
Chemical family: dicarboximide; *N*-phenylphthalimide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
flumiclorac acid



flumiclorac pentyl ester



Molecular formula: *Acid* $C_{16}H_{13}ClFNO_5$; *Pentyl ester* $C_{21}H_{23}ClFNO_5$
Molecular weight: *Acid* 353.73 g/mole, *Pentyl ester* 423.87 g/mole
Description: Beige, powdered solid, halide odor
Density: 0.9 μg/mL (20 C) (pentyl ester)
Melting point: 88.9-90.1 C
Boiling point: NA
Vapor pressure: 1.33 x 10^{-5} Pa (22.4 C)
Stability: Unstable in strong acid or strong base; Stable at 54 C for 14 d; not strongly degraded by UV light
Solubility:
water 0.189 mg/L (25 C):
organic solvents g/100 mL (25 C):

acetone 59	methylene chloride 288
acetonitrile 58.9	*n*-octanol 1.6
n-hexane 0.328	NMP 134
methanol 4.78	tetrahydrofuran 69.7

pK_a: NA
K_{ow}: 97,720 (20 C)

HERBICIDAL USE

Flumiclorac is being developed for control of certain broadleaf weeds such as velvetleaf; lambsquarters, common ragweed, pigweed spp., and spotted spurge in soybeans and corn. It can be applied POST at 30.2-90.4 g ai/ha in soybeans and POST at 30.2-45.2 g ai/ha or POST-directed at 60.3 g ai/ha in corn.

USE PRECAUTIONS

Fire hazard: Technical grade and RESOURCE are non-flammable. The flash point is 68 C.
Corrosiveness: Technical grade and RESOURCE are non-corrosive.
Storage stability: Technical grade and RESOURCE are stable under normal conditions.
Cleaning glassware/spray equipment: Through cleaning is recommended because flumiclorac is active at low concentrations and residues in the spray tank could be redissolved in a subsequent tank load, therefore, causing injury when applied POST to susceptible crops.
Emergency exposure: Flush eyes with water for at least 15 min; hold eyelids open. Wash skin with soap and water. If RESOURCE is ingested, drink water or milk and obtain medical advice, do not induce vomiting unless directed to do so by medical personnel.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14.
Symptomology: Symptoms may appear within 1 d under bright sunlight and include wilting and bleaching. Leaves then become brown, desiccated, and necrotic.
Absorption/translocation: Readily absorbed into leaves with little to no basipetal translocation in the phloem to the roots. Under good growing conditions, flumiclorac is rainfast 1 h after application.
Metabolism in plants: Soybeans and corn degrade flumiclorac more rapidly than does velvetleaf.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Resistance is due to a deletion in the PPO gene.

BEHAVIOR IN SOIL

Sorption: Strongly absorbed to both clay and OM
K_{oc} and K_d: NA. Flumiclorac degrades too rapidly to measure K_{oc} and K_d
Transformation:
Photodegradation: Half-life is 3-4 d in water and 1-2 d on soil; degradation products are further degraded by light, releasing CO_2

Other degradation: Half-life for non-microbial hydrolysis is 4.2 d at pH 5, 19 h at pH 7, and 6.6 min at pH 9.

Persistence: Extremely labile with half-lives ranging from <1 to 6 d; no rotational crop restrictions

Field experiments: Half-lives were <1 d in a silty loam soil in Mississippi; 5.8 d in a loam in Iowa; 4.8 d in a loamy sand in North Carolina; 1.4 d in a silt loam in Kentucky.

Lab experiments: Half-life was 0.48-4.4-d in a loamy sand with pH 6.8-7.1

Mobility: Does not leach; no residues observed below 7.5 cm in field studies. Runoff is not anticipated due to rapid breakdown and strong sorption to soil.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flumiclorac pentyl ester unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat and mouse, >5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.94 mg/L; Skin irritation rabbit, none; Skin sensitivity, guinea pig, no; Eye irritation rabbit, slight

RESOURCE EC: Oral LD_{50} rat, 3600 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 5.51 mg/L; Skin irritation rabbit, moderate; Skin sensitivity, guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, mouse: NOEL 125 mg/kg/d; slight anemia; enlargement of liver in male

90-d dietary rat: NOEL 67 mg/kg/d; increased liver and kidney weights

90-d dietary, dog: NOEL 10 mg/kg/d; slight decrease in body weight gain

21-d dermal, rat: NOEL 1000 mg/kg/d; no effects

Chronic toxicity:

18-mo dietary, mouse: NOEL 32 mg/kg/d; slight anemia in male; not oncogenic

24-mo dietary, rat: NOEL 35 mg/kg/d; increased liver and kidney weight; not oncogenic

12-mo dietary, dog: NOEL 100 mg/kg/d; reduced body weight gain in male; blood chemistry changes; increased liver to body weight ratio

Teratogenicity:

Rat: NOEL >1500 mg/kg/d

Rabbit: NOEL fetal 800 mg/kg/d, maternal 499 mg/kg/d; death in pregnant dams at 800 mg/kg/d

Reproduction:

Rat: Systemic NOEL maternal 10 mg/kg/d, fetal 14 mg/kg/d; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Mouse micronucleus, negative; In vitro CHO, negative without metabolic activation, weak positive with activation

DNA damage/repair: UDS, negative

Wildlife:

Bobwhite quail, oral LD_{50} >2259 mg/kg; 8-d dietary LC_{50} >5620 mg/kg; Mallard duck 8-d dietary LC_{50} >5620 mg/kg; Honey bee oral LD_{50} >106 μg/bee; Daphnia 48-h LC_{50} >38 mg/L; Bluegill sunfish 96-h LC_{50} 17.4 mg/L; Rainbow trout 96-h LC_{50} 1.1 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Pentyl 2-chloro-4-fluoro-5-aminopheoxyacetate is treated with 3,4,5,6-tetrahydrophthalic anhydride to obtain the pentyl ester of flumiclorac.

Purification of technical: NA

Analytical methods: NA

Historical: Discovered by Sumitomo Chemical Company, Ltd. In 1981. U.S. field tests were initiated in 1986. Developed in the U.S. by Valent USA Corporation, U.S. patents 4,670.046 (1987), 4,770,695 (1988), and 4,938,795 (1990). EPA registration is anticipated in 1994 for use in corn and soybeans.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Valent; Sumitomo

Reference(s):

1. Duke, S.O. et al. 1991. Weed Sci. 39:465.
2. Lee and Duke. 1994. Abstr. Weed Sci. Soc. Am. 34:52.

flumioxazin

CAS #: 103361-09-7

14(E)

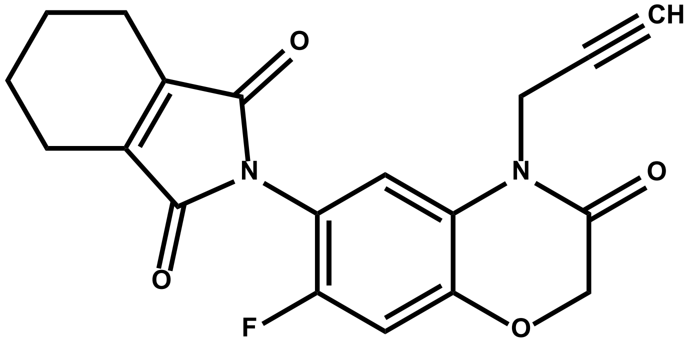
2-[7-fluoro-3,4-dihydro-3-oxo-4-(2-propynyl)-2H-1,4-benzoxazin-6-yl]-4,5,6,7-tetrahydro-1H-isoindole-1,3(2H)-dione

NOMENCLATURE

Common name: flumioxazin (ANSI, ISO, WSSA)
Other name(s): V-53482, S-53482 (code names), flumizin
Chemical name: N-(7-fluoro-3,4-dihydro-3-oxo-4-prop-2-ynyl-2H-1,4-benzoxazin-6-yl)cyclohex-1-ene-1,2-dicarboxamide (IUPAC)
Trade name(s): SUMISOYA; VALOR®
Chemical family: dicarboximide; *N*-phenylphthalimide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
flumioxazin



Molecular formula: $C_{19}H_{15}FN_2O_4$
Molecular weight: 354.34 g/mole
Description: Yellowish-brown, odorless
Density: 1.51 g/mL (20 C)
Melting point: 201.8 – 203.8 C
Boiling point: NA
Vapor pressure: 3.21×10^{-4} Pa
Stability: Stable at room temperature
Solubility: In water,1.79 mg/L (25 C)
pK$_a$: None (non-ionizable)
K$_{ow}$: log K_{ow} = 2.55 (20 C)

HERBICIDAL USE

Flumioxazin is used preemergence for broadleaf weed control in soybeans and peanuts. In soybean conventional-tillage herbicide programs, flumioxazin controls problem broadleaf weeds such as common ragweed, common lambsquarters, velvetleaf, pigweed, black nightshade, tall and common waterhemp, and prickly sida. Flumioxazin aids rapid burndown and offers residual control (4 to 6 weeks) of broadleaf weeds including common ragweed, common lambsquarters and velvetleaf in no-till and reduced-tillage herbicide programs in soybeans.

USE PRECAUTIONS

Fire hazard: Technical and formulated flumioxazin are non-flammable and non-explosive.
Corrosiveness: Formulated products are non-corrosive to containers.
Storage stability: Good stability. Store in cool, dry place and avoid excess heat. Store in original containers only. Keep out of reach of children and animals. Do not contaminate water, food or feed by storage or disposal.
Cleaning glassware/spray equipment: Clean glassware and equipment with a solution of soap and water. Avoid contamination of water by cleaning of equipment or disposal of wastes. Large spills should be covered to prevent dispersal.
Emergency exposure: If ingested, drink 1-2 glasses of water. Do not induce vomiting or give anything by mouth to an unconscious individual. Contact a medical doctor. If inhaled, remove to fresh air. If breathing discomfort occurs, contact a medical doctor. For skin and eye exposure wash with plenty of soap and water or flush with water for at least 15 min. If irritation occurs or persists get medical attention.
Incompatibilities: Flumioxazin has been found to be physically compatible with most commercially available herbicides.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Plants emerging from soils treated with the herbicide flumioxazin become necrotic and die shortly after exposure to sunlight. Foliar contact with flumioxazin causes rapid desiccation and necrosis of exposed plant tissues.
Absorption/translocation: Flumioxazin is taken up by the roots and foliage of treated plants. Shoot-root soil placement studies indicate that flumioxazin is absorbed primarily by the roots of treated plants following soil applications. Symplastic phloem movement is assumed to be limited, because of the rapid foliar desiccation caused by this herbicide.
Metabolism in plants: Flumioxazin is believed to be rapidly metabolized in tolerant plants such as soybeans and peanuts, leading to a number of metabolic transformations. Details about the exact metabolic reactions transforming flumioxazin are not available.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Development of weed resistance to this herbicide has not been observed.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: Flumioxazin is not susceptible to photodegradation once applied to soil. However, flumioxazin is susceptible to photodecomposition and has a half-life of 3.2 d in an aquatic system.
Other degradation: Based on laboratory tests, loss of flumioxazin in soil appears to be primarily by microbial

degradation. The half-life or aerobic soil metabolism of flumioxazin is 11.9 to 17.5 d. The hydrolytic degradation of flumioxazin in soil water has a half-life of 3.4 to 5.1 d (pH 5.0); 21.4-24.6 h (pH 7.0) and 14.6-22.0 min (pH 9.0) for flumioxazin in solution.

Persistence: Not persistent in soil

Mobility: Based on column leaching studies and the short aerobic soil half-life, the potential for flumioxazin or its degradation products to leach in field agricultural soil is low.

Volatilization: Not susceptible to volatility once applied to soil

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade and formulated flumioxazin.

Acute toxicity:

WP formulation: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >0.969 mg/L; Primary eye irritation rabbit, minimal clearing in 48 h; Skin irritation rabbit, slight at 72 h; Skin sensitization guinea pig, negative

Subchronic and Chronic toxicity:

Technical flumioxazin has been tested extensively in rats, mice and dogs. Results from these studies show that this herbicide is not carcinogenic. Adverse effects observed in animals exposed to high doses of technical flumioxazin for long periods of time included effects on blood, liver and kidney.

Teratogenicity:

Flumioxazin (technical) produced adverse effects on the offspring of rats exposed during pregnancy. However, it did not produce any adverse effects on the offspring of rabbits exposed during pregnancy.

Reproduction:

Reproduction toxicity was observed in a two-generation study with rats exposed to high levels of flumioxazin.

Mutagenicity:

Flumioxazin (technical) does not present a genetic hazard

Wildlife:

Flumioxazin is practically nontoxic to bees and avian species. It is slightly to moderately toxic to freshwater fish and moderately to highly toxic to aquatic invertebrates.

Bobwhite quail oral $LD_{50,}$ >2250 mg/kg; 8-d dietary $LD_{50,}$ >5620 mg/kg; Mallard duck oral $LD_{50,}$ >2250 mg/kg; 8-d dietary, LD_{50} >5620 mg/kg; Honey bee acute contact, LD_{50} >105 mg/bee; Daphnia 48-h EC_{50}, >6 mg/L; Bluegill sunfish 96-h $LC_{50,}$ >21 mg/L; Rainbow trout 96-h $LC_{50,}$ 2.3 mg/L; Oyster shell deposition $EC_{50,}$ 2.8 mg/L; Sheepshead minnow $LC_{50,}$ 2.8 mg/L; Mysid shrimp $LC_{50,}$ >0.23 mg/L.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Flumioxazin was introduced in 1989 by the Valent USA Corporation.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry Source(s): Valent

fluometuron

CAS #: 2164-17-2 $7^{(C_2)}$

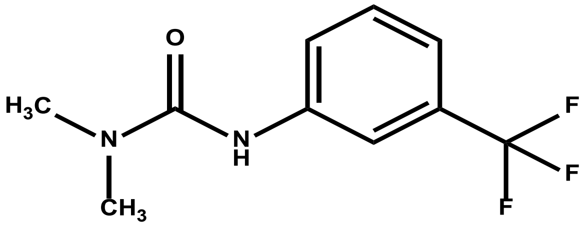
N,*N*-dimethyl-*N*'-[3-(trifluoromethyl)phenyl]urea

NOMENCLATURE

Common name: fluometuron (ANSI, BSI, ISO, WSSA)
Other name(s): C-2059; 1,1-dimethyl-3-(α,α,α-trifluoro-*m*-tolyl)urea (IUPAC); 1,1-dimethyl-3-(3-trifluoromethylphenyl) urea; 3-(*m*-trifluoromethylphenyl)-1,1-dimethylurea
Trade name(s): METURON®; COTORAN®; COTORAN® 4L; COTORAN® 80 DF
Chemical family: phenylurea; substituted urea; urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
fluometuron



Molecular formula: $C_{10}H_{11}F_3N_2O$
Molecular weight: 232.21 g/mole
Description: White crystalline solid, odorless
Density: 0.41 g/mL (20 C)
Melting point: 163-164.5 C
Boiling point: ~280 C (1.013×10^5 Pa)
Vapor pressure: 6.7×10^{-5} Pa (20 C); 1.2×10^{-4} Pa (25 C); 3.3×10^{-4} Pa (30 C); 1×10^{-3} Pa (40 C); 4.4×10^{-4} (50 C); 9.5×10^{-2} Pa (75 C); 1.3 Pa (100 C); 13 Pa (125 C); 100 Pa (150 C). Henry's Law constant, 2.6×10^{-9} atm m^3/mole
Stability: Hydrolyzes slowly at pH 1 (half-life is 580 d at 20 C)
Solubility:
water 110 mg/L (22 C)
organic solvents g/100 mL (20 C):
acetic acid 5
acetone 10.5
benzene 0.274
chloroform 2
dichloromethane 2.3
dimethylformamide soluble
ethanol soluble
n-hexane 0.011
isopropanol 4.7
methanol 11
toluene 0.24
pK_a: None (non-ionizable)
K_{ow}: 242 (25 C)

HERBICIDAL USE

Fluometuron can be used PPI at 1.8 kg ai/ha and PRE or POST at 1.12-2.24 kg ai/ha in cotton for control of many broadleaf and grass species, including barnyardgrass, crabgrass spp., fall panicum, foxtail spp., goosegrass, broadleaf signalgrass, cocklebur, Florida pusley, morningglory spp., lambsquarters, prickly sida, common ragweed, Sesbania, sicklepod, smartweed spp., and spurge spp. It can be applied in water or liquid fertilizer.

USE PRECAUTIONS

Fire hazard: All products are dry or aqueous and are non-flammable.
Corrosiveness: All products are non-corrosive
Storage stability: Stable for several years; not harmed by freezing. Decomposed by UV light
Cleaning glassware/spray equipment: Wash glassware with strong detergent and water. Flush equipment with water after removing nozzle tips and screens (clean these separately with detergent and water).
Emergency exposure: May cause eye, nose, and throat irritation. If ingested, nausea and vomiting may result; drink 1-2 glasses of water and induce vomiting or lavage stomach. No specific antidote is available, but ingestion of a slurry of activated charcoal can help inactivate the herbicide. Give a saline laxative and supportive therapy.
Incompatibilities: Fluometuron application after application of a systemic insecticide can cause crop injury; compatible with most other pesticides and fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Injury begins as interveinal chlorosis of the leaves, followed in susceptible plants by increasing chlorosis and necrosis. Cotyledons may show chlorotic areas. Older leaves show more damage than new growth. Root growth is not affected.
Absorption/translocation: Readily absorbed by roots after soil application and translocated predominately by the xylem to the shoots. Foliar-applied fluometuron is not highly absorbed and is not appreciably translocated out of the treated leaf through the phloem.
Metabolism in plants: Fluometuron undergoes successive *N*-demethylation as the primary detoxification process in plants. Competitive or subsequent hydroxylation may occur allowing the formation of sugar conjugates. Hydrolysis of the urea to form the aniline is not a significant process. Polar metabolites in cotton also may form by oxidation of the trifluoromethyl group to the carboxylic acid. Rapid metabolism is an important means of selectivity in tolerant plant species.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:
K_{oc} and K_d: Average K_{oc} is 100 mL/g (2). K_{oc} 80 mL/g and K_d 1.13 mL/g for a clay with 2.4% OM, 55.2% clay, and pH 5.7; K_{oc} 35 mL/g and K_d 0.079 mL/g for a sand with 0.39% OM, 3.2% clay, and pH 5.9; K_{oc} 54 mL/g and K_d 0.248 mL/g for a sandy clay loam with 0.78% OM, 21.2% clay, and pH 7.1; K_{oc} 57 mL/g and K_d 0.15 mL/g for a sandy loam with 0.45% OM, 7.2% clay, and pH 6.1

Transformation:

Photodegradation: Stable in water at 25 C and pH 5, 7, or 9 under natural light. Half-life was 9.7 d on a sandy loam at 10-36 C under natural light; major photolysis product was the mono-*N*-demethylated metabolite [*N*-methyl-*N*′-[3-(trifluoromethyl)phenyl]urea]. Photodegradation losses are substantial when little or no rainfall is received soon after application, but are moderate to low with adequate rainfall.

Other degradation: Half-life was 189 d for aerobic microbial metabolism and 378 d for anaerobic microbial metabolsim in a sandy loam at 25 C; major degradation product under aerobic and anaerobic conditions was mono-*N*-demethylated fluometuron. Microbial metabolism is the most important contributor to field dissipation, but rates are moderate. Non-biological degradation is negligible at pH 5, 7, and 9.

Persistence: Average field half-life is 85 d (2); fluometuron residues often dissipate to non-detectable levels by 4 mo after application of labeled rates.

Field experiments: Half-lives in dissipation studies conducted in cotton and sampling at 0-15 cm: 103 d for a loamy sand with 0.9% OM and pH 6.4 in Georgia; and 171 d for a sandy loam with 1.3% OM and pH 7.3 in California. Application rate and weather conditions can significantly impact half-life.

Mobility: In field experiments conducted in cotton grown in Georgia and California, no quantifiable fluometuron residues (LOD = 10 mg/kg) were found below 30 cm

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fluometuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 6416 mg/kg; Dermal LD_{50} rabbit, >10,000 mg/kg; 4-h inhalation LC_{50} rat, >2 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

COTORAN 4L: Oral LD_{50} male rat, 4960 mg/kg; female rat, 2870 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat, >2.5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

COTORAN DF: Oral LD_{50} rat, 1841 mg/kg; Dermal LD_{50} rabbit, >3038 mg/kg; 4-h inhalation LC_{50} rat, >2 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary rat: NOEL 7.5 mg/kg/d (100 mg/kg); liver, kidney, and spleen effects at 1000 and 10,000 mg/kg

90-d dietary dog: NOEL 15 mg/kg/d (400 mg/kg); liver, kidney, and spleen effects at 4000 mg/kg.

21-d dermal, rabbit: NOEL 1000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 1.2 mg/kg/d (10 mg/kg); conjunctival effects and reduced body weight gain at 500 and 2000 mg/kg; not carcinogenic

24-mo dietary, rat: NOEL 19 mg/kg/d (300 mg/kg); liver, kidney, and spleen changes; slight decrease in several hematological parameters at 1000 mg/kg; not carcinogenic

12-mo dietary, dog: NOEL 10 mg/kg/d (400 mg/kg); body weight, liver, kidney, and hematological effects at 7000 mg/kg

Teratogenicity:

Rat: NOEL 10 mg/kg/d; not teratogenic; maternal toxicity with secondary developmental effects at 100 and 1000 mg/kg/d

Rabbit: NOEL 10 mg/kg/d; not teratogenic; maternal toxicity with secondary developmental effects at 100 mg/kg/d

Reproduction:

Rat: NOEL 10 mg/kg; not a reproductive toxin; spleen changes at 300 and 1000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Chinese hamster/nucleus anomaly, negative

DNA damage/repair: Rat hepatocytes, negative; Human fibroblasts, negative

Wildlife:

Bobwhite quail oral $LD_{50,}$ >2150 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Japanese quail 8-d dietary LC_{50}, 4620 mg/kg; Mallard duck oral LD_{50}, 2974 mg/kg; 8-d dietary LC_{50}, 4500 mg/kg; Ringneck pheasant 8-d dietary LC_{50}, 3150 mg/kg; Daphnia 48-h LC_{50}, 54 mg/L; Bluegill sunfish 96-h LC_{50}, 48 mg/L; Carp 96-h LC_{50}, 170 mg/L; Catfish 96-h LC_{50}, 55 mg/L; Rainbow trout 96-h $LC_{50,}$ 30 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Alkylamination of the appropriate aromatic isocyanate

Purification of technical: Confidential

Analytical methods: Crop samples are extracted by reflux in NaOH which converts fluometuron and its metabolites to 3-trifluoromethylaniline (TFMA). TFMA is steam distilled and residues are cleaned up on a silica SepPak. Residues of TFMA are determined by GC using N/P detection and expressed as fluometuron equivalents. Soil samples are extracted by shaking with 80% methanol. Residues are partitioned into dichloromethane, cleaned up on a Grade V alumina column, and determined by normal phase HPLC with UV detection. Fluometuron in technical samples and formulated products is determined by GC using FID.

Historical: First reported in 1964 (1). British patent 914,779 and Belgian patent 594,227.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Agriliance; Griffin; Riverside/Terra, Adama

Reference(s):

1. Counselman, C. J. et al. 1964. Proc. South. Weed Control Conf. p. 189.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

fluoroglycofen

carboxymethyl 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoate

CAS # Acid: 77501-60-1
Ethyl ester: 77501-90-7

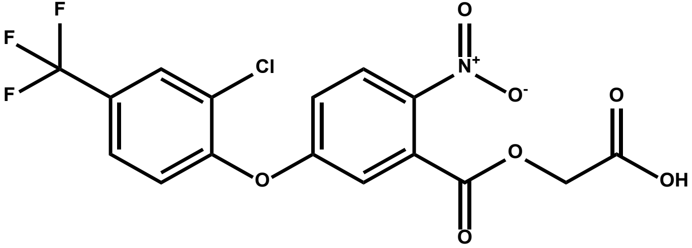
NOMENCLATURE

Common name: fluoroglycofen (ANSI, BSI, ISO, WSSA)
Other names: benzofluorfen; fluoroglicofene; fluoroglycofen-ethyl; RH-0265; *O*-[5-(2-chloro-α,α,α-trifluoro-*p*-tolyloxy)-2-nitrobenzoyl]glycolic acid (IUPAC); ethoxycarbonylmethyl 5-[2-chloro-4-(trifluoromethyl)-phenoxy]-2-nitrobenzoate; 2-ethoxy-2-oxoethyl 5-[2-chloro-4 (trifluoromethyl)phenoxy]-2-nitrobenzoate
Trade name(s): COMPETE®
Chemical family: diphenylether; nitrodiphenylether; nitrophenylether

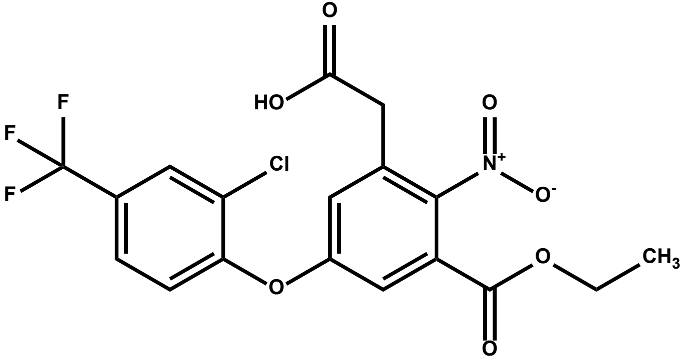
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

fluoroglycofen acid



fluoroglycofen ethyl ester



Molecular formula: *Acid* $C_{16}H_9ClF_3NO_7$; *Ethyl ester* $C_{18}H_{13}ClF_3NO_7$
Molecular weight: *Acid* 419.70 g/mole; *Ethyl ester* 447.75 g/mole
Description: Dark amber solid, musty odor
Density: 1.01 g/mL (25 C)
Melting point: 65 C
Boiling point: NA
Vapor pressure: $<1.33 \times 10^{-2}$ Pa
Stability: Rapidly degraded by UV light in aqueous suspension
Solubility:
water <1 mg/L (25 C)
>50 g/100 mL (25 C) in most organic solvents
pK_a: *Acid* NA; *Ethyl ester* None (non-ionizable)
K_{ow}: 2.7 (pH 7, 2 C), 15.1 (pH 4, 22 C)

Fluoroglycofen can be applied POST at 15-40 g ai/ha in cereal crops for control of several broadleaf weeds such as catchweed bedstraw, speedwell spp., *Viola* tricolor, and *Matricaria* spp. It currently is not registered in the U.S.

USE PRECAUTIONS

Fire hazard: COMPETE 20 WP is dry and non-flammable
Corrosiveness: COMPETE 20 WP is non-corrosive
Storage stability: No special storage problems under normal conditions
Cleaning glassware/spray equipment: Wash or flush with water
Emergency exposure: Wash skin with soap and water and flush eyes with water for at least 15 min; consult a physician if irritation persists. If ingested, dilute by drinking 2 glasses of water; call a physician.
Incompatibilities: May be incompatible with certain fertilizer solutions

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Rapid foliar necrosis and dessication
Absorption/translocation: Readily absorbed by foliage. Fluoroglycofen translocates very little following either root or foliar applications.
Metabolism in plants: Rapidly detoxified in tolerant species by de-esterification to 4-trifluoromethyl-2-chloro-3'-(carboxy) methoxy carbonyl-4'nitro-dephenyl) ether and 4-trifluoromethyl-2-chloro-3'carboxy-4'nitro-diphenyl ether followed by conjugation with glutathione or homoglutathione.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Readily absorbed to soil.
K_{oc} and K_f: K_{oc} 1364 mL/g and K_f 7.5 mL/g for adsorption, and K_f 0.41 mL/g for desorption in a sand with 0.55% organic carbon; K_{oc} 323 mL/g and K_f 3.84 mL/g for absorption, and K_f 13.1 mL/g for desorption in a silt loam with 1.19% organic carbon; K_{oc} 441 mL/g and K_f 7.41 mL/g for adsorption, and K_f 8.05 mL/g for desorption in a sandy loam with 1.68% organic carbon, K_{oc} 2208 mL/g and K_f 5.78 mL/g for adsorption, and K_f 2.14 mL/g for desorption in a clay with 0.26% organic carbon.
Transformation:
Photodegradation: Degrades rapidly and extensively in aqueous solution exposed to light.
Other degradation: Rapidly degraded by soil microbes
Persistence: Half-life is <1 wk for PRE applications, and 2-3 wk for POST applications
Mobility: Slight to moderate mobility depending on soil
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flucoroglycofen ethyl ester unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1500 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation $LC_{50,}$ NA; Skin irritation rabbit, slight; Skin sensitize Guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, mouse: NOEL, 1.5 mg/kg/d (10 mg/kg)
90-d-dietary, rat: NOEL 1 mg/kg/d (20 mg/kg)
90-d-dietary dog: NOEL 10 mg/kg/d (320 mg/kg)
28-d dermal; rabbit: NOEL <180 but > 10 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 1.5 mg/kg/d (10 mg/kg); liver tumors at 7.5 mg/kg/d (50 mg/kg)
24-mo dietary, rat: NOEL 1 mg/kg/d (20 mg/kg)
12-mo dietary, dog: NOEL 10 mg/kg/d (320 mg/kg)

Teratogenicity:

Rat and rabbit: NOEL NA; not teratogenic

Reproduction:

Rat: NOEL NA; no reproductive effects

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative
Structural chromosome aberration: *In vivo* and *in vitro* cytogenetics, negative
DNA damage/repair: Unspecified test, negative
Mammalian cell transformation: Unspecified test, negative

Wildlife:

Bobwhite quail oral $LD_{50,}$ >1075 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck 8-d dietary LC_{50}, >5000 mg/kg; Honey bee topical LD_{50}, >100 μg/bee; Daphnia 48-h $LC_{50,}$ 30 mg/L; Bluegill sunfish 96-h LC_{50}, 1.6 mg/L; Rainbow trout 96-h LC_{50}, 23 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React sodium 5-(2-chloro-4-(trifluoromethyl(phenoxy)-2-nitrobenzoate with ethyl monochloroacetate

Purification of technical: NA

Analytical methods: Analyzed by gas chromotography

Historical: Developed by Rohm and Haas Company. Fluoroglycofen is not registered in the U.S.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry Source(s): Dow AgroSciences

Reference(s):

1. Duke, S.O. et al. 1991. Weed Sci. 39:465.
2. Lee and Duke. 1994. Abstr. Weed Sci. Soc. Am. 34:52.

flupyrsulfuron-methyl-sodium

CAS #: 144740-54-5 **$2^{(B)}$**

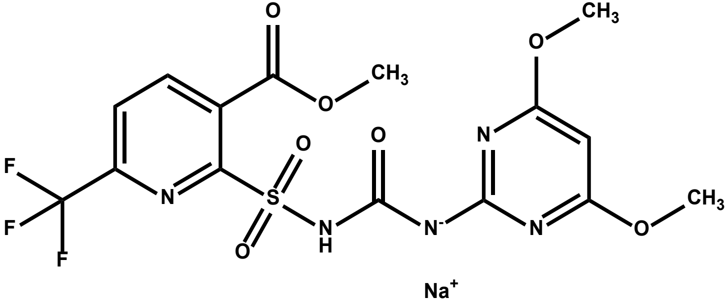
sodium salt of methyl 2-[[[[(4,6-dimethoxy-2-pyrimidinyl) amino]carbonyl]amino]sulfonyl]-6-(triflurromethyl)-3-pyridinecarboxylate

NOMENCLATURE

Common name: flupyrsulfuron-methyl-sodium (ISO)
Other name(s): DPX-KE459; flupyrsulfuron-methyl; sodium (4,6-dimethoxypyrimidin-2-yl)[({[3-(methoxycarbonyl)-6-(trifluoromethyl)pyridine-2-yl]sulfonyl}amino)carbonyl] azanide (IUPAC)
Trade name(s): LEXUS XPE; LEXUS MILLENIUM
Chemical family: sulfonylurea; pyrimidinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
flupyrsulfuron-methyl-sodium



Molecular formula: $C_{15}H_{13}F_3N_5NaO_7S$
Molecular weight: 465.36 g/mole
Description: Brown color
Relative density: NA
Melting point: 165-170 C
Boiling point: NA
Vapor pressure: $<10^{-8}$ Pa (25 C)
Stability: Stable
Solubility: 63 mg/L (pH 5, 25 C); 600 mg/L (pH 6, 25 C)
pK_a: 4.9 (weak acid)
K_{ow}: 0.96 (pH 5, 25 C); 0.11 (pH 6, 25 C)

HERBICIDAL USE

Flupyrsulfuron-methyl-sodium is a short residual sulfonylurea herbicide for the control of *Alopercus mynsuroides* (blackgrass), *Apera spica-venti* (windgrass) and select broadleaf weeds in cereal.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: Non-corrosive
Storage stability: Stable at normal storage conditions
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth of susceptible plants is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by slow, general foliar chlorosis and necrosis.
Absorption/translocation: Mobile in both the xylem and the phloem
Metabolism in plants: Tolerant species including wheat and *Avena fatua* metabolize flupyrsulfuron-methyl very rapidly (DT_{50} = 2 h) while sensitive species metabolize much more slowly (DT_{50} ~ 20 h). Flupyrsulfuron-methyl is metabolized in wheat and *Avena fatua* via a glutathione(GSH)-mediated cleavage of the sulfonylurea linkage. The gluthatione conjugate undergoes further transformation through hydrolysis. In *Phalaris minor*, the major metabolite resulted from *O*-demethylation of pyrimidinyl methoxy group.
Non-Herbicidal biological properties: None known
Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes.

BEHAVIOR IN SOIL

Sorption: K_{oc} ranged from 15 – 23 mL/g
Transformation: Flupyrsulfuron-methyl is rapidly degraded in aerobic soil under laboratory conditions with DT_{50} = 8-26 d and DT_{50} under field conditions of 6-11 d. Bridge contraction, cleavage of the sulfonylurea bridge, and *O*-demethylation are the major degradation products.
Mobility: Negligible
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flupyrsulfuron unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.8 mg/L (max. attainable conc.); Skin irritation rabbit, no; Skin sensitization guinea pig, no; Eye irritation rabbit, no

Mutagenicity:
Gene mutation: CHO/HGPRT, negative
Structural chromosome aberration: CHO, negative; Rat bone marrow, negative
DNA damage/repair: Primary rat hepatocytes/ UDS, negative

Wildlife:
Bobwhite quail oral LD_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, 721 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >820 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

fluridone

CAS #: 59756-60-4 **12$^{(F_1)}$**

1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]-4(1*H*)-pyridinone

NOMENCLATURE

Common name: fluridone (ANSI, BSI, ISO, WSSA).

Other name(s): ELI-171; 1-methyl-3-phenyl-5-(α,α,α-trifluoro-*m*-tolyl)-4-pyridone (IUPAC)

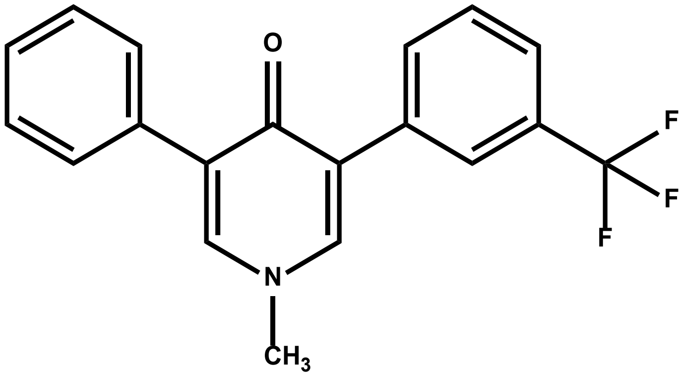
Trade name(s): SONAR®

Chemical family: None generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

fluridone



Molecular formula: $C_{19}H_{14}F_3NO$

Molecular weight: 329.32 g/mole

Description: White crystalline solid

Density: Loose 0.358 g/mL, packed 0.515 g/mL

Melting point: 154-155 C

Boiling point: Decomposes before boiling

Vapor pressure: 4.33×10^{-5} Pa (25 C)

Stability: Decomposes at 200 - 219 C

Solubility:

water 12 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C)
chloform >1 *n*-hexane <0.05
diethyl ether >0.1 methanol >1
ethyl acetate >0.5

pK_a: None (non-ionizable)

K_{ow}: 74 (20 C)

HERBICIDAL USE

Fluridone is an aquatic herbicide applied at 0.06-0.09 mg ai/L in pounds, 0.075-0.15 mg ai/L in lakes and reservoirs, or at 2.24 kg ai/ha of treated surface in drainage canals, irrigation canals, and rivers. It can be applied to the water surface or subsurface, or as a bottom application just above the hydrosoil. Fluridone controls most submerged and emerged aquatic plants including bladderwort, coontail, elodea, watermilfoil, naiad, pondweeds, hydrilla, and paragrass.

USE PRECAUTIONS

Fire hazard: All formulated products are non-flammable.

Corrosiveness: All formulated products are non-corrosive.

Storage stability: The product SONAR is stable for 36 mo at room temperature and for 9 mo at 5 C. SONAR is not damaged by freezing.

Cleaning glassware/spray equipment: Clean glassware with soap and water or a solvent; rinse equipment with water.

Emergency exposure: Flush eyes or skin with water, get medical attention if irritation persists. If ingested, drink 1-2 glasses of water and induce vomiting; call a physician or poison control center.

Incompatibilities: Compatible with water of any hardness; fluridone can be tank mixed with many other herbicides

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme phytoene desaturase in carotenoid biosynthesis. (more details on page 14)

Symptomology: Symptoms appear in 7-10 d as white (chlorotic) or pink growing points. Under optimum conditions, 30-90 d are required before weeds are controlled.

Absorption/translocation: Fluridone is systemic and is absorbed from the water by plant shoots and from the hydrosoil by roots. In cotton, a tolerant species, fluridone is taken up by the roots, but with little or no translocation into the shoots. In susceptible species, root-absorbed fluridone is translocated readily into the shoot (3).

Metabolism in plants: Fluridone is not metabolized appreciably in terrestrial plants (2).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Strongly absorbed to soil OM. OM content of terrestrial soil determines the rate of fluridone required for herbicidal activity. Fluridone adsorption/desorption coefficients correlate well with soil OM content. Fluridone is more strongly absorbed to sediments in aquatic environments at lower pH.

K_{oc} and K_d: Average K_{oc} is 1000 mL/g (7), but values range from ~ 350-2460 mL/g; K_{oc} = 350 mL/g and K_d = 3 mL/g for a loamy sand with 1.5% OM and pH 8.1; K_{oc} = 1000 mL/g and K_d = 6 mL/g for a sand with 1% OM and pH 6.5; K_{oc} = 1000 mL/g and K_d = 11 mL/g for a clay loam with 1.9% OM and pH 7.4; K_{oc} = 460 mL/g and K_d = 11 mL/g for a silty clay loam with 4.1% OM and pH 5.7; K_{oc} = 1100 mL/g and K_d = mL/g for a loam with 2.6% OM and pH 5.7

Transformation:

Photodegradation: Half-life is 22-55 h in deionized water. In aquatic environments, fluridone appears to be degraded principally by photolysis, although microbes and aquatic vegetation also may contribute (5). Photolysis rate may be affected by geographic location, application date, water depth, turbidity, weather, and weed cover, all of which may affect sunlight penetration of the water.

Other degradation: 1-methyl-2-(4-hydroxyphenyl)-5-[3-trifluoromethyl]-4[1*H*]-pyridinone is a minor metabolite in water and hydrosoil. In the lab, 1,4-dihydro-1-methyl-4-oxy-5-[3-trifluoromethyl)phenyl]-3-pyridinone was a major hydrosoil metabolite, but has not been identified in the hydrosoil of small ponds under natural conditions. Fluridone is not degraded by the hydrolysis (9).

Persistence: Average half-life is ~20 d in aerobic pond water, 9 mo in anaerobic pond water, and ~90 d in the hydrosoil. Fluridone adheres to sediments, but gradually desorbs into the water and then is subject to photodegradation.

Mobility: Not applicable in most cases because fluridone is applied to water. Fluridone leaches slowly in soil column leaching studies.

Volatilization: No losses

Formulation effects: SONAR SRP (pellets) generally degrades more slowly in water than does SONAR (aqueous suspension).

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fluridone unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat and mouse, >10,000 mg/kg, dog, >500 mg/kg, cat, >250 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >4.12 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

SONAR: Oral LD_{50} rat, >0.5 mg/kg; Dermal LD_{50} rabbit, >2 mg/kg; 1-h inhalation LC_{50} rat, >11 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

SONAR SRP: Oral LD_{50} rat, >500 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, mouse: NOEL 9.3 mg/kg/d

90-d dietary, rat: NOEL 53 mg/kg/d

90-d dietary, dog: NOEL 200 mg/kg/d

Chronic toxicity:

12-mo dietary, mouse: NOEL 11.4 mg/kg/d

24-mo dietary, mouse: 11.6 mg/kg/d; not carcinogenic

12-mo dietary, rat: NOEL 0.4 mg/kg/d

24-mo dietary, rat: NOEL 8.5 mg/kg/d; not carcinogenic

12-mo dietary, dog: NOEL 150 mg/kg/d

Teratogenicity:

Rat: NOEL 200 mg/kg/d; not teratogenic

Rabbit: NOEL 750 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 121 mg/kg/d (2000 mg/kg); not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Rat dominant lethal, negative; SEC, negative

DNA damage/repair: SEC, negative

Wildlife:

Bobwhite quail LD_{50}, >2000 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; 1-generation reproduction NOEL, >1000 mg/kg; Mallard duck 8-d dietary LC_{50}, >5000 mg/kg; 1-generation reproduction NOEL, >1000 mg/kg; Earthworm LC_{50} in soil, >102.6 mg/kg; Honey bee oral LD_{50}, >362.6 μg/bee; Daphnia 48-h LC_{50}, 6.3 mg/L; Bluegill sunfish 96-h LC_{50}, 14.3 mg/L; Rainbow trout 96-h LC_{50}, 11.7 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: The crude mixture is dissolved in 3A ethanol, carbon treated, and crystallized to yield purified fluridone.

Analytical methods: Plant and tissue samples are extracted with methanol. Tissue extracts are hydrolyzed with 2N HCl, purified by liquid-liquid partitioning and column chromatography, and measured by reverse phase HPLC with UV detection. Soil samples are extracted with boiling 2N NaOH: methanol (1:1), purified by alumina and XAD 2-column chromatography, and measured by reverse phase HPLC with UV detection (8, 10, 11, 12).

Historical: First described as a herbicide in 1976 (6). Introduced in Syria in 1977 by Eli Lilly & Company; British patent 1,521,092; introduced in the U.S. in 1986 as SONAR A.S., SONAR 5P, and SONAR SRP

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Dow AgroSciences; SePRO

Reference(s):

1. Bartels and Watson. 1978. Weed Sci. 26:198.
2. Berard, D. F. et al. 1978. Weed Sci. 26:252.
3. Marquis, L. Y. et al. 1981. Weed Sci. 29:229.
4. Sandmann and Böger. 1989. Pages 25-44 in P. Böger and G. Sandmann, eds., Target Sites of Herbicide Action. CRC Press, Boca Raton, FL.
5. Saunders and Mosier. 1983. J. Agri. Food Chem. 31:237.
6. Waldrep and Taylor. 1976. J. Agric. Food Chem. 24:1250.
7. Wauchope, R. D. et al. 1992. Environ. Contam. Toxicol. 123:1.
8. West, S.D. 1978. J. Agric. Food Chem. 26:644.
9. West, S. D. et al. 1983. J. Agric. Food Chem. 31:579.
10. West and Burger. 1980. J. Assoc. Offic. Anal. Chem. 63:1304.
11. West and Day. 1981. J. Assoc. Offic. Anal. Chem. 64:1205.
12. West and Day. 1986. J. Assoc. Offic. Anal. Chem. 69:856.

flurochloridone

CAS #: 61213-25-0 **$12^{(F_1)}$**

3-chloro-4-(chloromethyl)-1-[3-(trifluoromethyl)phenyl]-2-pyrrolidinone

NOMENCLATURE

Common name: fluorochloridone (BSI, draft E-ISO, draft F-ISO); flurochloridone (WSSA)

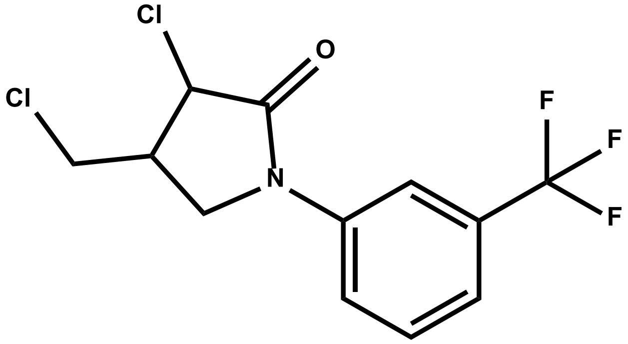
Other name(s): (3*RS*,4*RS*,3*RS*,4*RS*)-3-chloro-4-chloromethyl-1-(α,α,α-trifluoro-*m*-tolyl)-2-pyrrolidinone (in ratio 3:1) (IUPAC)

Trade name(s): RACER®; RAINBOW RIDER

Chemical family: None generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *flurochloridone*



Molecular formula: $C_{12}H_{10}Cl_2F_3NO$

Molecular weight: 312.12 g/mole

Description: Light peach colored solid

Density: 1.52 g/mL (20 C)

Melting point: 55-57 C(cis isomer); 81-83 C (trans isomer); 55.6-79 C (1:3 cis:trans)

Boiling point: 212.5 C (1.33 x 10^{-3} Pa)

Vapor pressure: 4.4 x 10^{-4} Pa

Stability: NA

Solubility:

water 35.1 mg/L (distilled); 20.4 mg/L (pH 9, 25 C)
ethanol (20 C):
100 g/L kerosene:<5 g/L
Readily soluble in:
Acetone, chlorobenzene, xylene

pK_a: None (non-ionizable)

K_{ow}: log K_{ow} =3.36

HERBICIDAL USE

Preemergence control of *Stellaria media,*. *Veronica hederifolia*, *Viola arvensis* in winter wheat & rye; *Amaranthus*, *Portulaca oleracea* & *Solanum nigrum* in cotton; *Galium, S. nigrum* and *Veronica persica* in potatoes and a wide range of weeds in sunflowers. Rate ranges from 500-750 g/ha.

USE PRECAUTIONS

Fire hazard: Exothermic decomposition was detected at 190-210 C.

Corrosiveness: NA

Storage stability: Keep container tightly closed in a cool, well-ventilated place. Decomposition will occur at elevated temperatures.

Emergency exposure: On ingestion, wash mouth out with water and seek medical advice. Do not induce vomiting. On eye contact, rinse with water for at least 15 min and seek medical advice.

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme phytoene desaturase in the carotenoid biosynthesis pathway (more details on page 14)

Symptomology: Foliage of sensitive plants bleach or turn white

Absorption/translocation: Absorbed by roots, stems and coleoptiles

Metabolism in plants: Rapidly metabolized by oxidation and conjugation to form numerous minor metabolites

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 680-1300 mL/g

Transformation:

Other degradation: Does not biodegrade in water.

Persistence: Half-life is 9-70 d; rapid degradation in soil

Mobility: Low

Volatilization: Low

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flurochloridone unless otherwise indicated.

Acute toxicity:

Oral LD_{50} for male rats, 4000 mg/kg; female rats, 3650 mg/kg; Dermal LD_{50} for rabbits, >5000 mg/kg; Skin irritation rabbit, none; Eye irritation rabbit, none; Skin sensitization guinea pigs, none

Chronic toxicity:

24-mo dietary, rat: NOEL 100 mg/kg diet male rats; 400 mg/kg diet female rats; 12-mo dietary, dog

Teratogenicity:

Rat: NOEL 2.3 mg/kg/day

Mutagenicity:

Gene mutation: Genotoxicity negative

Wildlife:

Bobwhite quail LD_{50}, >2000 mg/kg; Mallard ducks Dietary LC_{50} (5-d) and Bobwhite quail, >5000 mg/kg; Rainbow trout LC50 (96-h), 3 mg/L; Bluegill sunfish, 6.7 mg/L, Daphnia EC_{50} (48-h), 5.1 mg/L; Bees LD_{50}, >100 mg/bee

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: Reported herbicide by F. Pereiro in 1982. Commercialized in 1985 by Stauffer Chemical Co (Now Syngenta).

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Syngenta Crop Protection

fluroxypyr

[(4-amino-3,5-dichloro-6-fluoro-pyridinyl)oxy]acetic acid

CAS # Acid: 69377-81-7
Meptyl ester: 81406-37-3
Butometyl ester: 154486-27-8

$4^{(O)}$

NOMENCLATURE

Common name: fluroxypyr (acid form); (meptyl ester) fluroxypyr-meptyl;

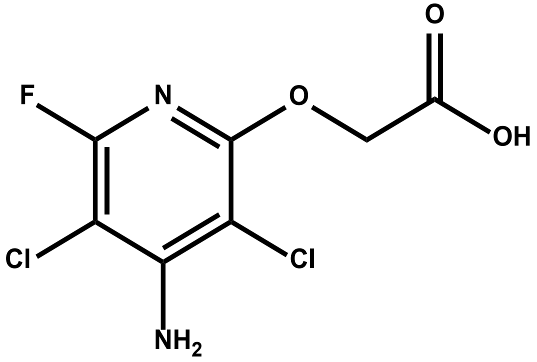
Other name(s): DOWCO 433 (acid form) 4-amino-3,5-dichloro-6-fluoro-pyridyloxyacetic acid (IUPAC); (meptyl ester)(*RS*)-1-methylheptyl 4-amino-3,5-dichloro-6-fluoro-2-pyridyloxyacetate

Trade name(s): ADVANCE; ATTAIN; STARANE®; VISTA®; WIDEMATCH®, PRESTIGE®; RETRIEVE®; TOMIGAN®

Chemical family: pyridine; pyridinyloxyacetic acid

CHEMICAL AND PHYSICAL PROPERTIES

fluroxypyr acid



Molecular formula: *Acid* $C_7H_5Cl_2FN_2O_3$; *Meptyl ester* $C_{15}H_{21}Cl_2FN_2O_3$

Molecular weight: *Acid* 255.03 g/mole; *Meptyl ester* 367.25 g/mole;

Description: Both the ester and acid forms of fluroxypyr are known to display herbicidal activity

Density: *Acid* 1.76 g/mL; *Meptyl ester* 1.3 g/mL (20 C)

Melting point: *Acid* 206 C; *Meptyl ester* (57.5 C)

Vapor pressure: *Acid* 5 x 10^{-5} Pa (25 C); *Meptyl ester* 2 x 10^{-5} Pa (25 C)

Stability: Avoid temperatures above flash point (for STARANE 200, 47 C)

Solubility:

Acid

water (pH 6.95, 20 C) 4000 mg/L

organic solvents g/100 mL (20 C):

acetone	6.2
acetonitrile	0.82
ethyl acetate	1.21
1-octanol	0.27

Ester

water (pH 7.0, 20 C) 0.0136 mg/L

organic solvents g/100 mL (20 C)

acetone	330
acetonitrile	250
n-heptane	6.23
dichloromethane	250
ethyl acetate	250
1-octanol	22

pK_a: *Acid* 3.04 (weak acid); *Meptyl ester* None (non-ionizable

K_{ow}: log K_{ow} *Acid* -1.5 (pH 7); *Meptyl ester* 4.57 (pH 5); 5.04 (pH 7)

HERBICIDAL USE

Fluroxypyr offers a novel mode of action and is efficacious against many broadleaf and sulfonylurea-resistant weeds. In North America, the current use is in small grains, fallow cropland and rights-of-way. Fluroxypyr was registered in Canada in 1996 as STARANE and in combination with 2,4-D Ester, as ATTAIN Herbicide Tank-Mix; in 1997, PRESTIGE Herbicide was registered in Canada as a co-package. In 1998, U.S. registrations are STARANE and VISTA.

USE PRECAUTIONS

Emergency exposure: Wash skin with soap and water, if irritation develops seek medical attention. Irrigate eyes with water for at least 15 min and seek medical attention. DO NOT induce vomiting if ingested.

Irritant: Meptyl ester: mild eye irritant; essentially non-irritating to skin

BEHAVIOR IN PLANTS

Mechanism of action: Disruption of plant cell growth; appears to act as an auxin similar to indoleacetic acid (IAA), a natural plant growth hormone. Also interferes with plant's ability to metabolize nitrogen and produce enzymes. (more details on page 12)

Symptomology: Fluroxypyr is a broad spectrum selective auxin-mimicking (growth regulator) foliar applied herbicide. In susceptible plant species, it induces an epinastic response, (i.e. stimulation of cell elongation and premature senescence, particularly in meristematic tissue) leading to cessation of normal growth and death, with observable leaf-curling. Plants die in days or weeks.

Absorption/translocation: There is rapid absorption by foliage of growing plants and may also be taken up by roots. It displays little soil activity. Upon conversion from ester to acid form, fluroxypyr is systemic and readily translocated throughout the plant via the phloem and to a lesser extent the xylem for distribution throughout entire plant, including meristems.

Resistance: To date weed resistance has not been observed.

Metabolism in Plants: Once hydrolyzed to the acid form, the rate of formation of conjugates (*N*-glucosyl) determines the phytotoxic response.

BEHAVIOR IN SOIL

Sorption:

K_{oc} *Acid* 39 mL/g to 71 mL/g over 4 soils; *Ester* 20000 mL/g

K$_d$: *Acid* in OECD test ranged from 0.78 to 1.34 mL/g

Transformation:

Photodegradation: Not an important dissipation mechanism

Aerobic soil metabolism: Upon application there is rapid conversion of the ester to acid form. The half-life range of total fluroxypyr (acid and ester) in soils is one to four weeks in laboratory studies. Microbial metabolism is the primary degradation mechanism in soil; the dichloropyridinol and methoxypyridine are known soil metabolites.

Aquatic metabolism: DT$_{50}$ range from 4 to 14 d for total fluroxypyr

Field dissipation: Half-lives for North American sites range from 11 to 38 d for total fluroxypyr (acid and ester). In the field, the ester form is no longer significant after one to two weeks. In Europe, DT$_{50}$ values of <3 d have been observed for the ester and 34 to 68 d for the acid form.

Mobility: Field dissipation study under representative uses indicated little movement. No fluroxypyr was detected past 30 cm at 7 sites (Canadian and US). European field lysimeter work indicates both forms are not mobile and are unlikely to contaminate groundwater.

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Studies on absorption, distribution, excretion and metabolism in mammals: Studies that have been conducted to investigate the pharmokinetics and metabolism of fluroxypyr, concluded that the ester form is rapidly hydrolyzed and the fate of the hydrolysis products is independent of whether they were given as the ester, or not. Fluroxypyr was extensively absorbed and then rapidly excreted principally unchanged in the urine. Also no significant differences in general toxicity between acid and ester forms have been observed.

Acute Toxicity:

Oral LD$_{50}$ rat: *Acid,* >2000 mg/kg, *Meptyl ester,* >5000 mg/kg; Dermal LD$_{50}$ rat: *Acid and Meptyl ester,* >2000 mg/kg; Eye Irritation: *Meptyl ester*, mild irritation; Skin Irritation: *Meptyl ester*, no irritation; Skin Sensitization: *Meptyl ester*, no sensitization; Acute inhalation (4-hour) LC$_{50}$ rat: *Meptyl ester,* >1 mg/L (1000 mg/m^3; maximum attainable concentration)

Subchronic:

90-d dietary ICR (Crj;CD-1) mouse: *Acid* NOEL males, >1,342 mg/kg/day, females, >1,748 mg/kg/day; 90-d dietary Wistar rat: *Acid* NOEL, 80 mg/kg/day; 90-d dietary Fischer 344 rat: *Acid* NOEL, 700 mg/kg/day; NOAEL, 1000 mg/kg/day; *Meptyl ester,* 1000 mg/kg/day; 28-d dietary dog: NOAEL, $\geq$ 50 mg/kg/day (range finding for chronic study)

Subacute dermal rabbit: NOAEL 1000 mg/kg/day (the highest dose tested)

Mutagenicy: *Acid* and *Meptyl ester* the weight of evidence of thorough testing indicates a lack of genetic toxicity; Ames test: *Acid* Negative

Chronic Toxicity and Carcinogenicity:

18-mo dietary, mouse: *Acid* Chronic toxicity NOEL 300 mg/kg/day; no evidence of oncogenicity at any dose level including 1000 mg/kg/day (highest dose tested)

24-mo dietary, Fischer 344 rat: *Acid* NOEL 100 mg/kg/day for males and 500 mg/kg/day for females; no evidence of oncogenicity at any dose level including 1000 mg/kg/day (highest dose tested)

12-mo dietary, dog: *Acid* NOEL 150 mg/kg/day (highest test dose)

Reproductive and Developmental Toxicity:

Wistar rat: *Acid* no effect on fertility or reproductive performance over two generations - NOAEL 500 mg/kg/day (highest dose tested)

Sprague-Dawley rat: *Acid* parental NOEL for systemic effects 100 mg/kg/day males and 500 mg/kg/day in females; NOEL for reproductive effects 750 mg/kg/day in males and 1000 mg/kg/day in females (highest dose tested); Neonatal NOEL 500 mg/kg/day

CD rat teratology: *Acid* maternal NOAEL 250 and fetal NOAEL 500 mg/kg/day, *Meptyl ester* maternal and developmental toxicity 300 mg/kg/day. No evidence of teratogenicity with either form of the compound

Rabbit teratology: *Acid* NOEL 250 mg/kg/day, *Meptyl ester* NOEL maternal and fetal toxicity 500 mg/kg/day. No evidence of teratogenicity with either form of the compound

Wildlife:

Acid: Quail acute oral LD$_{50}$, >2000 mg/kg; Duck acute oral LD$_{50}$, >2000 mg/kg; Dietary quail LC$_{50}$, >5000 mg/kg; Dietary duck LC$_{50}$, >5620 mg/kg; Bluegill 96-h LC$_{50}$, >14.3 mg/L; Rainbow trout 96-h LC$_{50}$, >100 mg/L; 21-d NOEC, 100 mg/L; Daphnia magna 48-h EC$_{50}$, >100mg/L; 21-d NOEC, 56 mg/L; *Menidia beryllina* 96-h LC$_{50}$, 40 mg/L; Grass shrimp 96-h LC$_{50}$, >120 mg/L; *Pseudokirchneriella subcapitata* green algae 120-h EC$_{50}$, 51.3 mg/L (cell numbers) with NOEL 34.2 mg/L; honeybee acute contact LD$_{50}$, >25 µg a.i./bee with NOEL, $\geq$25 µg a.i./bee

Meptyl ester: Quail acute oral LD$_{50}$, >2000 mg/kg; Duck acute oral LD$_{50}$, >2000 mg/kg; Dietary quail LC$_{50}$, >5000 mg/kg; Dietary duck LC$_{50}$, >5620 mg/kg; Long-term reproductive quail LC$_{50}$, >1000 mg/kg; Long-term reproductive duck NOEL, 500 mg/kg; Bluegill 96-h LC$_{50}$, >620 µg/L (measured), >100 mg/L (applied); Rainbow Trout 96-h LC$_{50}$, >225 µg/L (measured), >100 mg/L (applied); Daphnia magna 48-h LC$_{50}$, >183 µg/L (measured), >100 mg/L (applied); Sheephead Minnow 96-hr LC$_{50}$, >86 µg/L (measured), > 100 mg/L (applied); Grass shrimp 96- LC$_{50}$, >135 µg/L (measured), >100 mg/L (applied); *Pseudokirchneriella subcapitata* green algae 96-h EC$_{50}$, >1.41 mg/L (cell numbers) NOEC, 0.199 mg/L; honeybee acute contact LD$_{50}$, >100 µg a.i./bee; earthworm LC$_{50}$, >1000 mg/kg

SYNTHESIS AND ANALYTICAL METHODS

Analytical methods: Analysis involves both acid- and base hydrolyses and allows for determination of total fluroxypyr, whether present as the ester, free acid or conjugates with detection by GC/MS. Small grains method has a limit of quantitation of 0.01 µg/g for grain and 0.05 µg/g for forage, straw and hay.

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences; UAP-Loveland Products

Reference(s):

1. Bergstrom, L. F., McGibbon, A. S., Day, S. R. and Snel, M. *Pestic. Sci.* 29, 405-417, 1990.
2. Lehmann, R., G. and Miller, J. R. *J. Chromatogr*. 485, 581-584, 1989.
3. Lehmann, R. G. and Miller, J. R. *Weed Research* 29, 385-389, 1989.
4. Lehmann, R. G., Lickly, L. S., Lardie, T. S., Miller, J. R. and Baldwin, W. S. *Weed Research* 31, 347-355, 1991. (EPA MRID#42137320)
5. Lehmann, R. G., Miller, J. R., Olberding, E. L., Tillotson, P. M. and Laskowski, D. A. *Weed Research* 30, 375-382, 1990.6. Lehmann, R. G., Miller, J. R., Olberding, E. L., Tillotson, P. M. and Laskowski, D. A. *Weed Research* 30, 383-388, 1990.
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8. Tonks, D. J. and Westra, P. *Weed Technology* 11, 270-276, 1997.
9. Friesen, L. F. and Morrison, I. N., Rashid, A. and Devine, M. D. *Weed Science* 41, 100-106, 1993.
10. Lym, R. G. *Weed Science* 40, 101-105, 1992.
11. Orfanedes, M. S. and Wax, L. M. *Weed Technology* 5, 782-788, 1991.
12. Orfanedes, M. S., Wax, L. M. and Liebl, R. A. *Weed Science* 41, 1-6, 1993.

flurtamone

CAS #: 96525-23-4 **12(F₁)**

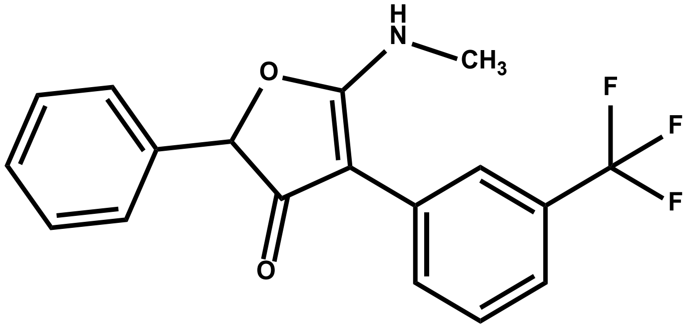
5-(methylamino)-2-phenyl-4-[3-(trifluoromethyl)phenyl]-3(2*H*)-furanone

NOMENCLATURE

Common name: flurtamone (ISO)
Other name(s): RE-40885, RO-40885; (*RS*)-5-methylamino-2-phenyl-4-(α,α,α-trifluro-*m*-tolyl)furan-3(2*H*)-one (IUPAC)
Trade name(s): BIZON®; CARAT®; CLINE®; DOLMEN®; NIKEYL®; BACARA®
Chemical family: furanone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
flurtamone



Molecular formula: $C_{18}H_{14}F_3NO_2$
Molecular weight: 333.31 g/mole
Description: Ivory powder
Density: NA
Melting point: 152-155 C
Boiling point: NA
Vapor pressure: NA
Stability: Stable but avoid concentrated acids or bases.
Solubility:
water, 35 mg/L (20 C)
soluble in acetone
dichloromethane methanol
slightly soluble in isopropanol
pK$_a$: None (non-ionizable)
K$_{ow}$: NA

HERBICIDAL USE

Flurtamone is used for pre-plant incorporated, preemergence or postmergence control of broadleaf and some grass weeds in small grains, peanuts, cotton, peas, and sunflowers at 250-375 g ai/ha.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Cleaning glassware/spray equipment: NA
Emergency exposure: Eyes: flush immediately with fresh water for at least 15 minutes. Skin: wash affected areas with soap and water. Ingestion: give water or milk to drink and seek medical advice.
Incompatibilities: Strong acids and bases

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme phytoene desaturase in carotenoid biosynthesis (more details on page 14)
Symptomology: Bleaching of stems and leaves of susceptible plant species.
Absorption/translocation: Absorbed by roots and foliage; translocated via the xylem
Metabolism in plants: Metabolized to more polar degradation products
Mechanism of resistance in weeds: No resistance has been reported

BEHAVIOR IN SOIL

Persistence:
Field experiments: DT$_{50}$ 4-8 weeks
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade flurtamone unless otherwise indicated.
Acute toxicity:
Oral LD$_{50}$ rat, >500 mg/kg; Dermal LD$_{50}$ rat, >5000 mg/kg; Irritation to skin rabbit, no; Eye irritation rabbit, transient
Chronic toxicity: NOEL 50 mg/kg daily
Mutagenicity: Non-mutagenic (Ames test)
Wildlife:
Bobwhite quail LC$_{50}$, >6000 mg/kg, Mallard ducks, 2000 mg/kg diet; Bluegill sunfish LC$_{50}$ (96 h), 11 mg/kg, Rainbow trout, 7 mg/L; LD$_{50}$ (48 h, contact), > 100 μg/bee
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

fluthiacet-methyl

CAS #: 117337-19-6

$14^{(E)}$

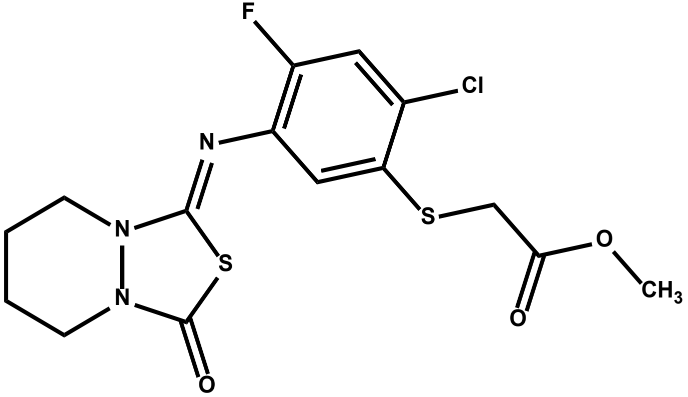
acetic acid, [[2-[chloro-4-fluoro-5-[(tetrahydro-3-oxo-1*H*,3*H*-[1,3,4]thiadiazolo[3,4-*a*]pyridazin-1-ylidene)amino] phenyl]thio]-, methyl ester

NOMENCLATURE

Common name: fluthiacet-methyl (ISO)
Other name(s): KIH-9201; methyl {2-chloro-4-fluoro-5-[(*EZ*)-5,6,7,8-tetrahydro-3-oxo-1*H*, 3*H*-[1,3,4]thiadiazolo[3,4-*a*] pyridazin-1-ylideneamino] phenylthio}acetate (IUPAC)
Trade name(s): APPEAL®; BLIZZARD®
Chemical family: imine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
fluthiacet-methyl



Molecular formula: $C_{15}H_{15}ClFN_3O_3S_2$
Molecular weight: 403.87 g/mole
Description: Dark amber solid, musty odor
Density: 0.431 g/mL (25 C)
Melting point: 104.6 C
Boiling point: NA
Vapor pressure: 3.45×10^{-7} Pa (20 C); 4.41×10^{-7} Pa (25 C)
Stability: Stable at room temperature and at 50 C in metal, glass or plastics containers
Solubility:
water 850 mg/L (25 C)
pK_a: None (Non-ionizable)
K_{ow}: 5870

HERBICIDAL USE

Fluthiacet-methyl can be applied POST at 3-15 g ai/ha in corn and soybeans for control of velvetleaf and certain other broadleaf weeds. It can also be applied alone or in combination with other harvest aids labeled for use on cotton. A surfactant or oil adjuvant is required for maximum efficacy. Fluthiacet-methyl has no soil activity.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Non-corrosive
Storage stability: Stable for more than three years at room temperature in the dark.
Cleaning glassware/spray equipment: NA
Emergency exposure: If ingested, drink 1-2 glasses of water and induce vomiting
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Leaves of susceptible plants become chlorotic and then desiccated and necrotic within 1-2 d. Corn and soybean leaves present at application may show slight speckling or bronzing, but subsequently emerging leaves are not affected. Fluthiacet residues in soil do not affect seedling emergence.
Absorption/translocation: Little foliar-absorbed fluthiacet translocates basipetally.
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Strongly absorbed to soil
Transformation:
Photodegradation: Rapidly degraded in water and on soil with half-lives of 4.9 and <0.5 d, respectively.
Persistence: Extremely short residual with a half-life of 1-2 d
Mobility: Slightly mobile
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fluthiacet-methyl unless otherwise indicated.
Acute toxicity:
LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, none; Skin sensitize guinea pig, no; Eye irritation rabbit, slight
5% WP: Oral LD_{50} rat, >5050 mg/kg; Dermal LD_{50} rabbit, >2.2 mg/kg; 4-h Inhalation LC_{50} rat, >5.3 mg/L; Skin irritation rabbit, slight; Skin sensitize guinea pig, no; Eye irritation rabbit, slight
Subchronic toxicity:90-d dietary, mouse: NOEL, 10 mg/kg; target organs were liver, spleen, and the blood-forming system
90-d-dietary, rat: NOEL 100 mg/kg; decreased body weight and weight gain; target organs were liver and the blood-forming system
90-d-dermal rat: NOEL >1000 mg/kg/d
Chronic toxicity:
12-mo dietary, dog: NOEL male, 2000 mg/kg, female, 1000 mg/kg; decreased body weight gain; liver and the

blood-forming system were target organs.

Teratogenicity:

Rat: NOEL 1000 mg/kg/d; no effects

Rabbit: NOEL maternal 1000 mg/kg/d, develop-mental >300 mg/kg/d and >1000 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL parental, 25 mg/kg; developmental, 500 mg/kg in a 2-generation study; liver toxicity and decreased weight and weight gain in parents at >500 mg/kg; reduced pup body weight and weight gain at 5000 mg/kg (highest dose); not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; Chinese hamster V79 cells, negative

Structural chromosome aberration: Rat hepatocytes/micronucleus tests, negative; Mouse bone marrow/micronucleus test, negative; Chinese hamster lung cells, positive at cytotoxic doses; CHO, a positive at cytotoxic doses; Human lymphocytes, positive at cytotoxic doses.

DNA damage/repair: Rat hepatocytes/auto-radiographic test, negative

Wildlife:

Bobwhite quail, oral $LD_{50,}$ >2250 mg/kg; 8-d dietary $LC_{50,}$ >5620 mg/kg, reproductive NOEC, 100 mg/kg; Mallard duck, oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50} >5620 mg/kg, reproductive NOEC, 100 mg/kg; Honey bee topical $LD_{50,}$ >100 μg/bee; Daphnia, 48-h LC_{50}, >2.3 mg/L; life cycle NOEL 0.035 mg/L; Bluegill sunfish 96-h $LC_{50,}$ 0.14 mg/L; Fathead minnow early life stage NOEL 2.7 μg/L; Rainbow trout 96-h LC_{50}, 0.043 mg/L

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: A multi-step process beginning with 2-fluoroaniline

Purification of technical: NA

Analytical methods: Percentage active ingredient in fluthiacet-methyl technical is determined by reverse phase HPLC using a water-acetonitrile gradient.

Historical: Discovered and being developed by Kumiai Chemical Industry Co., Ltd. and Ihara Chemical Industry Co., Ltd.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): K-I Chemical USA Inc.

Reference(s):

1. Duke, S.O. et al. 1991. Weed Sci. 39:465.

fluxofenim

CAS #: 88485-37-4 **NC**

1-(4-chlorophenyl)-2,2,2-trifluoroethanone *O*-(1,3-dioxolan-2-ylmethyl)oxime

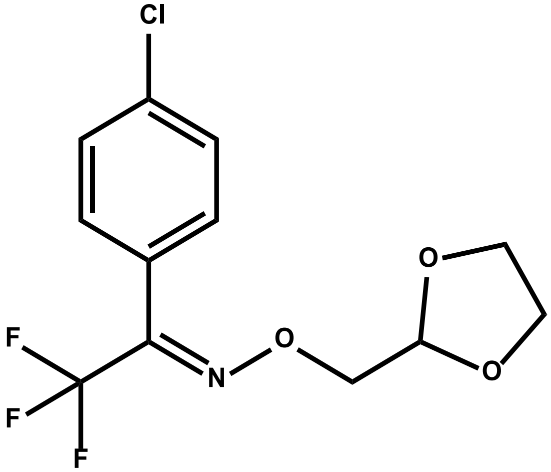
NOMENCLATURE

Common name: fluxofenim (ISO)
Other name(s): CGA-133205; 4′-chloro-2,2,2-trifluoroacetophenone (*EZ*)-*O*-1,3-dioxolan-2-ylmethyloxime (IUPAC)
Trade name(s): CONCEP® III
Chemical family: oxime

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

fluxofenim



Molecular formula: $C_{12}H_{11}ClF_3NO_3$
Molecular weight: 309.67 g/mole
Description: Colorless oil, mild odor
Density: 1.36 g/mL (20 C)
Melting point: NA
Boiling point: 1.33 x 10^1 Pa (94 C)
Vapor pressure: 3.9 x 10^{-2} Pa (20 C); 1.2 x 10^{-1} Pa (30 C); 3.3 x 10^{-1} Pa (40 C)
Stability: Slow exothermic decomposition at >200 C with strong exothermic decomposition at >300 C; Slowly degraded by UV light (<1% decomposition at >300 nm for 2 h); Stable to hydrolysis at pH 3-9 and 50 C
Solubility:
  water 300 mg/L (20 C)
  organic solvents (20 C):
  miscible in acetone
  dichloromethane
  methanol
  toluene
  cyclohexanone
  n-hexane
  n-octanol
  xylene
pK$_a$: None (non-ionizable)
K$_{ow}$: 7943

HERBICIDAL USE

Fluxofenin has no herbicidal activity but is used as a safener to protect sorghum from injury by chloroacetamide herbicides (such as *S*-metolachlor) applied PRE or PPI. It is applied as a seed treatment at 0.4 g ai/kg of seed, typically by placing seed in a fluxofenin/water slurry. Sorghum seed must be dried quickly after treatment to avoid significant imbibition. Good-germinating hybrids or seed lots typically show no loss in germination percentage following fluxofenin treatment; weaker-germinating hybrids or seed lots may germinate at slightly lower percentages.

USE PRECAUTIONS

Fire hazard: CONCEP III is combustible; flash point is 93.3 C.
Corrosiveness: CONCEP III is non-corrosive
Storage stability: Stable at room temperature; do not allow the mixture to freeze
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: May cause eye and skin irritation. Prolonged inhalation may cause headache, dizziness, breathing difficulty, or nausea. If ingested, drink 1-2 glasses of water and induce vomiting or lavage stomach. No specific antidote is available but ingestion of a slurry of activated charcoal may help inactivate the chemical. Treat symptomatically.
Incompatibilities: Do not mix with EC formulations of heptachlor. fluxofenin does not affect the efficacy of most herbicides.

BEHAVIOR IN PLANTS

Mechanism of action: Increases the detoxification rate of metolachlor and other chloroacetanilides by elevating glutathione *S*-transferase activity in sorghum (1, 2).
Symptomology: Fluxofenin is not phytotoxic and causes no observable injury.
Absorption/translocation: Absorbed primarily through the seed coat with some likely absorbed by the coleoptile during germination and early coleoptile growth. Translocation probably is unimportant in fluxofenin mode of action because the safener is absorbed by the germinating seed or the growing coleoptile is already close to the most important site of chloroacetamide herbicidal action near the coleoptilar node.
Metabolism in plants: NA
Non-antidotal biological properties: None known

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Persistence: NA
Mobility: NA
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fluxofenim unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 699 mg/kg; Dermal LD_{50} rabbit, 1554 mg/kg; 4-h inhalation LC_{50} rat, >1.2 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

CONCEP III: Oral LD_{50} rat, 943 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat, 4.17 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, slight.

Subchronic toxicity:

90-d dietary, rat: NOEL 0.7 mg/kg/d (10 mg/kg); liver effects at 150 and 300 mg/kg; kidney changes at ≥30 mg/kg

90-d dietary, dog: NOEL 20 mg/kg/d; liver, kidney, and thyroid effects in females at 40 mg/kg/d

21-d dermal, rabbit: NOEL 125 mg/kg/d; no systemic effects

Chronic toxicity: NA

Teratogenicity:

Rat: NOEL maternal 1 mg/kg/d, developmental 15 mg/kg/d; not teratogenic

Reproduction: NA

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Mouse micronucleus, negative

DNA damage/repair: Rat hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2000 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, 0.22 mg/L; Bluegill sunfish 96-h LC_{50}, 2.55 mg/L; Rainbow trout 96-h LC_{50}, 0.9 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Multistep condensation of trifluorochloroacetophenone with a halogenated dioxolane.

Purification of technical: Distillation from toluene

Analytical methods: Treated seeds are extracted by homogenization in methanol. Residues are determined by GC with flame ionization or electron capture detection. Fluxofenin is determined in technical samples and formulated products by GC with flame ionization detection.

Historical: Fluxofenin was synthesized by Ciba-Geigy Ltd. in Basel, Switzerland, and was first tested in 1982. U.S. patent 4,530,716.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Dean, J. V. et al. 1990. Plant Physiol. 92:467.
2. Gronwald, J. W. et al. 1987. Pestic. Biochem. Physiol. 29:66.

fomesafen

CAS # Acid: 72178-02-0
Na salt: 108731-70-0

14$^{(E)}$

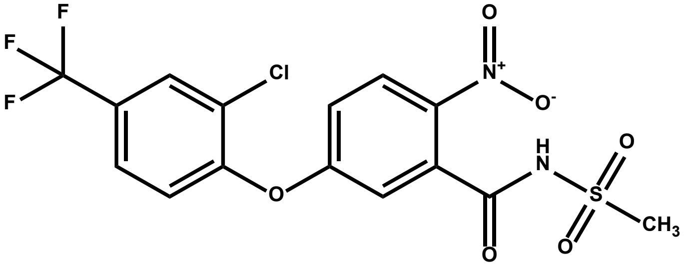
5-[2-chloro-4-(trifluoromethyl)phenoxy]-*N*-(methylsulfonyl)-2-nitrobenzamide

NOMENCLATURE

Common name: fomesafen (ANSI, BSI, ISO, WSSA)
Other name(s): formesafene; PP0-21; 5-(2-chloro-⟨α,α,α-trifluoro-p-tolyloxy)-*N*-mesyl-2-nitrobenzamide (IUPAC)
Trade name(s): REFLEX®; FLEX®; FLEXSTAR®; FUSIFLEX®; PREFIX®; ROBUST®, RUMBLE, TORMENT
Chemical family: amide; diphenylether; nitrodiphenylether; nitrophenylether

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
fomesafen acid



Molecular formula: *Acid* $C_{15}H_{10}ClF_3N_2O_6S$;
Na salt $C_{15}H_9ClF_3N_2NaO_6S$
Molecular weight: *Acid* 438.76 g/mole, *Na salt* 460.74 g/mole
Description: White crystalline solid
Density: 1.28 g/ml (20 C)
Melting point: 220-221 C
Boiling point: NA
Vapor pressure: 1.33×10^{-5} Pa (50 C)
Stability: Unstable in light; not readily hydrolyzed in acid or alkaline conditions; stable for >6 mo at 50 C
Solubility:

Acid
water ~50 mg/L (pH 7, 25 C); <1 mg/L (pH 1, 25 C)
organic solvents g/100 mL (25 C):
acetone 30
methanol 2.5
cyclohexanone 1
methylene chloride 1
dichloromethane 1
xylene 0.19
n-hexande 0.05

Sodium salt
water 600,000 mg/L (25 C)
organic solvents g/100 mL:
acetone 70 methanol 70
n-hexane ~0.0005 methylene chloride 0.4

pK_a: 2.7 (20 C) (weak acid) (4)
K_{ow}: 794 (pH 1)

HERBICIDAL USE

Formesafen can be applied POST at 0.28-0.42 kg ai/ha in soybeans to control many annual broadleaf weeds including morningglory spp., pigweed spp., jimsonweed, wild mustard, black nightshade, and ragweed spp.

USE PRECAUTIONS

Fire hazard: REFLEX and FLEX are aqueous and nonflammable
Corrosiveness: REFLEX and FLEX are non-corrosive under normal conditions
Storage stability: Store formulated products above 0 C to prevent freezing
Cleaning glassware/spray equipment: Wash equipment with detergent and rinse with water
Emergency exposure: If ingested, drink 1-2 glasses of water and induce vomiting; repeat until vomit is clear
Incompatibilities: Avoid acids

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Leaves of susceptible plants become chlorotic and then desiccated and necrotic within 1-3 d. Youngest expanded leaves of tolerant crops such as soybeans also may show chlorosis and necrosis, especially at higher rates. Sublethal rates may produce foliar "bronzing" usually on young expanded leaves. Droplet drift may cause bleached spots or flecks on leaves.
Absorption/translocation: Rapidly absorbed into leaves with minimal loss of activity when simulated rainfall occurred 1 h after application. Fomesafen is primarily mobile in the xylem. It may be absorbed through the root system.
Metabolism in plants: Soybean tolerance is due to rapid cleavage of the diphenylether bond, producing inactive metabolites.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Adsorption coefficients correlated approximately linearly with soil OM content across a range of soils.
K_{oc}: Average is 60 mL/g for the Na salt (4)
Transformation:
Photodegradation: Photodecomposes readily under relatively low sunlight intensities
Other degradation: Rapidly decomposed under anaerobic conditions
Persistence: Average field half-life is 100 d (4). Residues persist long enough to injure certain susceptible crops such as sugarbeets, sunflowers, and sorghum 1 yr after application.
Field experiments: Half-life in flooded soil was ≤ 8 wk
Lab experiments: Degraded rapidly under anaerobic

conditions with a typical half-life of <3 wk. Degraded slowly under aerobic conditions with a half-life of ~6-12 mo depending on soil characteristics

Mobility: Moderately mobile; in lab studies, mobility was similar to that of atrazine

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fomesafen acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1250-2000 mg/kg; Dermal LD_{50} rabbit, 1600 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, mild; Skin sensitize guinea pig, no; Eye irritation rabbit, mild

Fomesafen sodium salt technical: Oral LD_{50} female rat, 1499 mg/kg; Dermal LD_{50} female rat, >780 mg/kg; Skin irritation rabbit, slight; Eye irritation rabbit, moderate

REFLEX 2LC: Oral LD_{50} male rat, 8160 mg/kg; female rat, 6570 mg/kg; Dermal LD_{50} rabbit, >3.1 mg/kg

Subchronic toxicity:

90-d dietary, rat: NOEL 5 mg/kg/d

180-d-dietary, dog: NOEL ~30-40 mg/kg/d

Chronic toxicity:

24-mo dietary, rat: NOEL 100 mg/kg/d

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Fomesafen acid technical: Bobwhite quail oral LD_{50}, >2000 mg/kg; Mallard duck oral LD_{50}, >5000 mg/kg

REFLEX 2LC: Honey bee oral LD_{50}, >50 μg/bee, topical LD_{50}, >100 μg/bee; Bluegill sunfish 96-h LC_{50}, 6030 mg/L; Rainbow trout 96-h LC_{50}, 680 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: The appropriate acid chloride is reacted with methane sulfonamide

Purification of technical: NA

Analytical methods: Fomesafen and its derivatives can be analyzed in formulated products by HPLC with UV detection, in soils by HPLC, and in crop samples by TLC, HPLC, or NMR.

Historical: Herbicidal activity of fomesafen was first tested in the U.S. in 1978 by ICI Americas. Patent no. EP8416 was awarded to ICI Agrochemicals (now Syngenta Crop Protection). Fomesafen was first reported in 1983 (1).

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Adama, Syngenta Crop Protection

Reference(s):

1. Colby, S.R., et al. 1983. Proc. 10th Intern. Congr. Plant Prot. 1:295.
2. Duke, S.O. et al. 1991. Weed Sci. 39:465.
3. Lee and Duke. 1994. Abstr. Weed Sci. Soc. Am. 34:52.
4. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

foramsulfuron

CAS #: 173159-57-4 **$2^{(B)}$**

2-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-4-(formylamino)-*N,N*-dimethylbenzamide

NOMENCLATURE

Common name: foramsulfuron (ISO)

Other name(s): AEF-130060; 1-(4,6-dimethoxypyrimidin-2-yl)-3-[2-(dimethylcarbamoyl)-5-formamidophenylsulfonyl] urea (IUPAC)

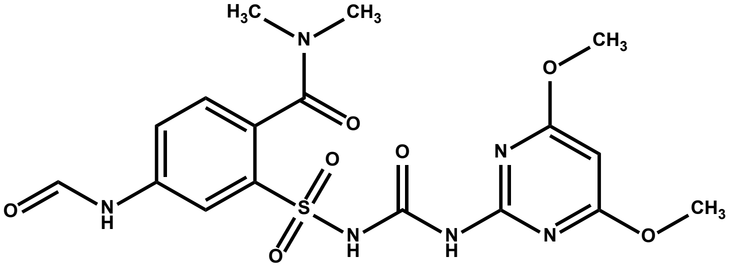
Trade name(s): EQUIP®; OPTION®; REVOLVER®; TRIBUTE®

Chemical family: pyrimidinylsulfonylurea; sulfonlyurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

foramsulfuron



Molecular formula: $C_{17}H_{20}N_6O_7S$

Molecular weight: 452.44 g/mole

Description: Light beige

Density: 1.44 g/mL (20 C)

Melting point: 202 C

Boiling point: NA

Vapor pressure: 4.2×10^{-11} Pa (20 C); 1.3×10^{-10} Pa (25 C); Henry's Law constant, 5.8×10^{-12} Pa m^3 mol^{-1}

Stability: Stable

Solubility: Water, 37.2 mg/L (pH 5, 20 C); 3293 mg/L (pH 7, 20 C); 945777 mg/L (pH 8, 20 C)

pK_a: NA

K_{ow}: 4.01 (pH 5.5 - pH 5.7)

HERBICIDAL USE

Foramsulfuron is under development as a postemergence grass herbicide for corn that has some control of small-seeded broadleaves. A second product, a mixture of foramsulfuron and iodosulfuron, will provide broad spectrum grass and broadleaf control, as well as control of some perennial weeds. Both provided good control of giant foxtail, common ragweed, pitted morningglory and Pennsylvania smartweed. Waterhemp control was poor with both herbicides.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.

Corrosiveness: Non-corrosive

Storage stability: Stable under normal storage conditions

Cleaning glassware/spray equipment: Wash with water and detergent.

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Growth of susceptible plants in inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by slow, general foliar chlorosis and necrosis.

Absorption/translocation: Mobile in both the xylem and the phloem

Metabolism in plants: Foramsulfuron undergoes hydrolysis of the sulfonylurea bridge and the formamide moiety.

Non-Herbicidal biological properties: None known

Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes.

BEHAVIOR IN SOIL

Sorption: Weakly sorbed to soils

Transformation:

Hydrolysis: Stable

Photodegradtion: Water- stable; soil - stable

Other degradation: Aerobic soil metabolism $t_{½}$ = 40 d; anaerobic soil metabolism $t_{½}$ =76 d

Persistence:

Field experiments: $t_{½}$ = 11-18 d

Mobility: Negligible

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade foramsulfuron acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal rabbit LD_{50}, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.04 mg/L (max. attainable conc.); Skin irritation rabbit, no; Skin sensitization guinea pig, no; Eye irritation rabbit, no

Subchronic toxicity:

90-day dietary, mice: NOEL 1002 mg/kg/d for males; 1178 mg/kg/d for females

Chronic toxicity:24-mo dietary, rats: NOAEL 849 mg/kg/d

Mutagenicity:

Gene mutation: CHO/HGPRT, negative

Structural chromosome aberration: CHO, negative; Rat bone marrow, negative

DNA damage/repair: Primary rat hepatocytes/ UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >5620 mg/kg; Daphnia, 48-h LC_{50}, 721 mg/L;

Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >820 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

fosamine

ethyl hydrogen (aminocarbonyl)phosphonate

CAS # Acid: 59682-52-9
Ammonium salt: 25954-13-6

27$^{(Z)}$

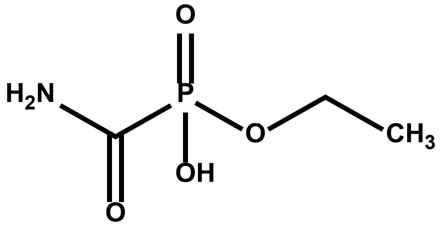
NOMENCLATURE

Common name: fosamine (ANSI, BSI, ISO, WSSA)
Other name(s): DPX 1108; ammonium ethyl carbamoylphosphonate; ethyl hydrogen carbomoylphosphonate (IUPAC)
Trade name(s): KRENITE®
Chemical family: organophosphorus

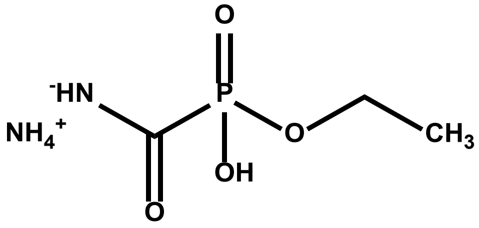
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

fosamine acid



fosamine ammonium salt



Molecular formula: *Acid:* $C_3H_8NO_4P$;
NH4 salt: $C_3H_{11}N_2O_4P$
Molecular weight: *Acid:* 153.07 g/mole;
NH4 salt: 170.11 g/mole
Description: White crystalline solid
Density: 1.33 g/mL
Melting point: 175 C
Boiling point: NA
Vapor pressure: 5.3×10^{-4} Pa (25 C)
Stability: Stable to UV light
Solubility:
water 1,790,000 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 0.024
benzene 0.035
chloroform 0.006
ethanol 0.95
n-hexane 0.013
methanol 12.6
pK_a: NA
K_{ow}: NA

HERBICIDAL USE

Fosamine can be foliar-applied at 9-54 kg ai/ha for brush control on non-crop land or for site preparation on land to be planted to conifers. It also can be applied in a spray-to-wet treatment using 1.78-3.55 kg ai/100 L water. An oil adjuvant may be added for maximum efficacy.

USE PRECAUTIONS

Fire hazard: KRENITE products are aqueous and nonflammable
Corrosiveness: KRENITE products are somewhat corrosive to brass or copper.
Storage stability: KRENITE products and spray tank solutions are stable. Dilute solutions decompose under acid conditions.
Cleaning glassware/spray equipment: Clean glassware with a detergent wash. Flush equipment with several changes of water after removing nozzle tips and screens (clean these parts separately).
Emergency exposure: Flush eyes or skin with water
Incompatibilities: Not normally used in combination with other pesticides

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Fosamine strongly inhibited mitosis in tissues of mesquite, but this may be a secondary effect (7).
Symptomology: In most woody plants, fosamine injury is not apparent before normal leaf senescence in the fall. However, leaf and bud development is severely or completely inhibited the following spring. Leaves that emerge appear abnormally small and spindly. Certain other plants such as pines and bindweed may show a response soon after application. On moderately susceptible to resistant species, suppression of terminal growth may occur.
Absorption: Penetration of fosamine into leaf tissue is generally slow, with less than 50% of the applied herbicide absorbed 7-8 d after application in black cherry, rhododendron, magnolia (5), blackberry (8), field horsetail (2), and multiflora rose (6). Retention and penetration is further reduced when fosamine is applied to very hairy leaf surfaces. Good penetration occurs, however, when fosamine is applied to young stems. The slow rate of fosamine absorption increases the potential for washoff by rainfall. Surfactants may increase fosamine penetration rate.
Translocation: Fosamine translocation occurs both symplastically and apoplastically, but is limited in most species examined. In blackberry, multiflora rose, and field horsetail, the herbicide initially translocated somewhat rapidly, accumulating to near maximum concentration in non-treated tissues 1 d after treatment. However, no significant increase in fosamine accumulation occurred thereafter. Field experience as well as limited translocation of fosamine in radioisotope studies supports the view that complete coverage of the plant is required for adequate control under field conditions. Tolerant species, such as rhododendron and magnolia, translocate less fosamine than more susceptible species (5), suggesting that translocation may be important to herbicide efficacy.
Metabolism in plants: Fosamine had an average half-life of 7 d when applied POST to pasture grasses and red clover

(1). The primary metabolite was carbamoylphosphonic acid (CPA) which reached a. maximum concentration after 2-4 wk. Carboxyphosphonic acid also was detected as a metabolite. No fosamine or its metabolites were found in pasture turf or clover 12 mo after treatment. Late summer application of fosamine to pin oak did not result in rapid decline of the herbicide because the plant went into dormancy shortly after treatment. In contrast, the half-life of foliar-applied fosamine in apple seedlings grown under greenhouse conditions was 2-3 wk.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 150 mL/g (9)

Transformation:

Photodegradation: Not appreciably degraded in water exposed to artificial or natural sunlight. Photosensitizers do not appear to accelerate fosamine photodegradation.

Other degradation: Rapidly decomposed by soil microbes. In lab tests with ^{14}C-carbamoyl-labeled fosamine ammonium salt at 4 and 20 mg/kg in two different soils, evolved $^{14}CO_2$ accounted for 45-75% of the original ^{14}C after 90-d incubations.

Persistence: Typical field half-life is 8 d (9)

Field experiments: Half-life was ~1 wk in Florida, Delaware, and Illinois. Half-life for complete dissipation of the fosamine molecule was 2-6 mo.

Lab experiments: Half-life was ~10 d in greenhouse studies (3, 4).

Mobility: In Florida, Delaware, and Illinois, there was little to no downward movement of fosamine or its degradation products because of rapid degradation.

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade fosamine ammonium salt unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 24,400 mg/kg; Dermal LD_{50} rabbit, >1683 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

KRENITE S: Oral LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50} male rat, 3.3 mg/L; female rat, 2.75 mg/L

Subchronic toxicity:

90-d dietary, rat: NOEL male 10,000 mg/kg (highest level tested)

2-wk dietary, rat: NOEL NA; no histopathologic evidence of cumulative toxicity at 2200 mg/kg/d in males

Chronic toxicity:

6-mo dietary, dog: NOEL 10,000 mg/kg

Teratogenicity:

Rat: NOEL maternal 350 mg/kg/d, fetal >3000 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 5000 mg/kg in a 2-generation study; no effects

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: *In vivo* cytogenetics, negative; *In vitro* cytogenetics, positive

Wildlife: NA

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React triethyl phosphate with methyl chloroformate and ammonia

Purification of technical: Recrystallization from 95% ethanol

Analytical methods: Residues in soil and plant tissue are measured as a silyl derivative using GC with phosphorus selective flame photometric detector (Du Pont, unpublished procedure).

Historical: Biological properties were first described in 1974 (10). Covered by U.S. patents 3,627,507 and 3,846,512 assigned to Du Pont Company.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

1. Chrzanowski, R. L. 1983. J. Agric. Food Chem. 31:223.
2. Coupland and Peabody. 1981. Weed Sci. 29:556.
3. Han, J. C. Y. 1979. J. Agric. Food Chem. 27:564.
4. Han and Krause. 1979. Soil Sci. 128:23.
5. Kitchen, L. M. et al. 1980. Weed Res. 20:285.
6. Mann, R. K. et al. 1986. Weed Sci. 34:830.
7. Morey and Dahl. 1980. Weed Sci. 28:251.
8. Richardson, R. G. 1980. Weed Res. 20:159.
9. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
10. Zoebisch, O. C. et al. 1974. Proc. Northeast. Weed Sci. Soc. 28:347.

glufosinate

2-amino-4-(hydroxymethylphosphinyl)butanoic acid

CAS # Acid (racemic mixture): 53369-07-6
Acid (unstated stereochemistry): 51276-97-2
Acid (*D*-isomer): 35597-44-5
Ammonium salt (unstated stereochemistry):
77182-82-2

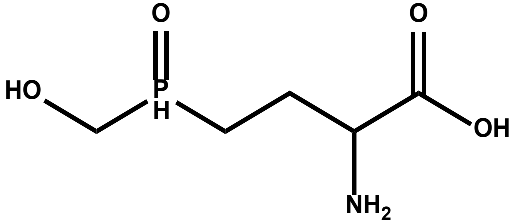
10$^{(H)}$

NOMENCLATURE

Common name: glufosinate (BSI, ISO, WSSA)
Other name(s): HOE 00661; HOE 39866; phosphinothricin; *DL*-homoalanine-4-yl-(methyl)-phosphinate; glufosinate-ammonium=ammonium (4-hydroxy(methyl)phophinoyl]-*DL*-homoalaninate or ammonium *DL*-homoalanin-4-yl(methyl) phosphinate (IUPAC)
Trade name(s): FINALE™; RELY®; IGNITE®; BASTA®
Chemical family: organophosphorus

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure ; *glufosinate acid*



Molecular formula: *Acid* $C_5H_{12}NO_4P$; NH_4 salt $C_5H_{15}N_2O_4P$
Molecular weight: *Acid* 181.13 g/mole; NH_4 salt 198.16 g/mole.
Description: White to light-yellow crystalline powder, slightly pungent odor
Density: 1.4 g/mL (20 C)
Melting point: 215 C
Boiling point: 99.5 C
Vapor pressure: 1.0 x 10^{-4} Pa (25 C)
Stability: Highly stable
Solubility:
water 1,370,000 mg/L (pH 7, 20 C)
organic solvents g/100 mL (20 C):
acetone 0.016
ethanol 0.065
ethyl acetate 0.014
n-hexane 0.02
toluene 0.014
pK_a: <2, 2.9, and 9.8
K_{ow}: NA

HERBICIDAL USE

Glufosinate can be applied POST at 0.35-1.7 kg ai/ha (0.32-1.56 kg ae/ha) in non-crop areas and as a directed spray in field-grown and container nursery stock. It is non-selective and controls a broad spectrum of annual and perennial grass and broadleaf weeds. Glufosinate also can be used in a spray-to-wet application at 1.41-3.75 g ai/L of water. Glufosinate can also be used in Liberty-Link crops such as corn and canola that have been genetically modified (see mechanism of resistance section) for broad spectrum POST weed control.

USE PRECAUTIONS

Fire hazard: IGNITE is combustible
Corrosiveness: Non-corrosive
Storage stability: Stable for 2 yr at 25 C
Cleaning glassware/spray equipment: Clean equipment with detergent or approved tank cleaners.
Emergency exposure: Flush eyes with water for at least 15 min. Wash skin with soap and water. If ingested, drink 1-2 glasses of water, induce vomiting, and seek medical attention. Phenobarbitol was an efficient therapeutic agent in animal antidote studies.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits glutamine synthetase activity and the production of glutamine (more details on pages 13)
Symptomology: Chlorosis and wilting usually occur within 3-5 d after application, followed by necrosis in 1-2 wk. Rate of symptom development is increased by bright sunlight, high humidity, and moist soil. Seedlings are not injured before emergence.
Absorption/translocation: Glufosinate requires a 6-h rain-free period after application for maximum efficacy. Little to no glufosinate is absorbed through the roots under field conditions because of rapid microbial breakdown. Glufosinate movement in xylem or phloem is limited.
Metabolism in plants: *D*-Glufosinate appears to be stable in plants (2), but *L*-glufosinate was metabolized to 4-methylphosphinico-2-oxo-butanoic acid, 3-methylphosphinico-propanic acid, and 4-methyl-phosphinico-2-hydroxybutanoic acid in tobacco, alfalfa, and carrots (1).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: A gene coding for phosphinothricin acetyl transferase activity was isolated from *Streptomyces hygroscopicus* and cloned into several crops species. This enzyme converts glufosinate to a non-phytotoxic acetylated metabolite (1) by transferring the acetyl group from acetyl-coenzyme A onto the amino group of glufosinate. The genetically engineered crops are thus able to rapidly detoxify glufosinate. The trait is inherited as a simple dominant allele.

BEHAVIOR IN SOIL

Sorption: Weakly absorbed to soil
K_{oc}: Average is 100 mL/g (estimated) (7)
Transformation: Rapidly degraded by microbes in soil or surface water to 3-methyl phosphinico-propionoic acid and ultimately to CO_2.
Persistence: Short soil residual life with a typical field half-life of 7 (d) (7).
Mobility: Highly mobile in soil. Despite high leaching potential glufosinate has been detected no deeper than 15 cm in field studies, presumably because of rapid microbial degradation.

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade glufosinate ammonium salt unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 2170 mg/kg; female rat, 1910 mg/kg; Dermal LD_{50} male rabbit, 1400 mg/kg; female rabbit, 1380 mg/kg; 4-h inhalation LC_{50} rat, 3.73 mg/L; Skin irritation rabbit, slight; Skin sensitization, NA; Eye irritation, NA

Subchronic toxicity: NA

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Japanese quail oral LD_{50}, >2000 mg/kg; Honey bee nontoxic; Rainbow trout 96-h LC_{50}, >320 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Contact Bayer CropScience

Historical: The ammonium salt of glufosinate was reported as an herbicide in 1981 (5). Glufosinate was introduced in Canada in 1993 and in Europe a few yr earlier, FINALE was introduced in 1994 in the U.S.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Dröge-Laser, W. et al. 1994. Plant Physiol. 105:159.
2. Dröge, W. et al. 1992. Planta 187:142.
3. Lea, P. J. et al. 1984. Phytochemistry 23:1
4. Sauer, H. et al. 1987. Naturforsch. 42C:270.
5. Schwerdtle, F. et al. 1981. Pflanzenkr. Pfanzenschutz. Sonderheft IX. P. 431.
6. Tachibana K. et al. 1986. J. Pestic. Sci. 11:33.
7. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1

glyphosate

N-(phosphonomethyl)glycine

CAS # acid: 1071-83-6

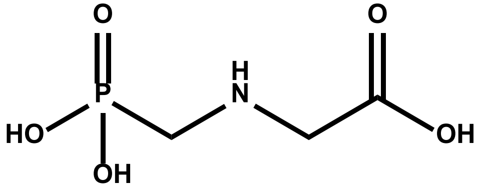
$9^{(G)}$

NOMENCLATURE

Common name: glyphosate (ANSI, BSI, ISO, WSSA)
Other name(s): ICIA0224; MONO0573; SC-0224; 2-(phosphonomethylamino)acetic acid; carboxymethylaminomethylphosphonic acid; sulfosate = trimethylsulfonium carboxymethylaminomethyl-phosphonate (IUPAC)
Trade name(s): ACCORD® CONCENTRATE; ACCORD® XRT; AQUAMASTER®; AQUANEAT®; BACKDRAFT®; CAMPAIGN®; DUPLIKATOR™ 5.5 PLUS; DURANGO™; EAGLE; EXTREME®; FALLOW MASTER®; FALLOW STAR®; FIELD MASTER®; FORZA™; GLY-FO; GLYFOS® AQUATIC; GLYFOS® PRO; GLYFOS® X-TRA; GLIFOSATO ESTRELLA; GLYPHOS XTRA®; DUPONT GLYPHOSATE VMF; GLYPHOSATE ORIGINAL; GLYPHOGAN™; GLYPHOMAX®; GLYPHOMAX PLUS®; GLYPRO®; GLYPRO PLUS®; GLYPHOSATE®; GLY STAR; HONCHO®; HONCHO® PLUS; IMITATOR® PLUS; LANDMASTER® BW; LANDMASTER® II; MIRAGE®; PIN-UP; POLADO® L; QUIKPRO®; RANGER PRO™; RATTLER®; RATTLER® PLUS; RAZOR®; READY MASTER ATZ®; RODEO®; ROUNDUP®; ROUNDUP® ORIGINAL; ROUNDUP® ORIGINAL RT; ROUNDUP® PRO CONCENTRATE; ROUNDUP® CUSTOM; ROUNDUP® PRO DRY; ROUNDUP® ULTRA; ROUNDUP® ULTRA RT; ROUNDUP® ULTRADRY; ROUNDUP® ULTRAMAX; ROUNDUP® ULTRAMAX II; ROUNDUP® D-PAK; ROUNDUP® WEATHERMAX; RT 3™; RT MASTER® II; SILHOUETTE®; STAPLE®PLUS; TOUCHDOWN®; TOUCHDOWN® PRO; WEEDOFF
Chemical family: organophosphorus

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure
glyphosate acid



Molecular formula: *Acid* $C_3H_8NO_5P$; *isopropylamine* (*IPA*) *salt* $C_6H_{17}N_2O_5P$; *trimethylsulfonium (TMS) salt* $C_6H_{16}NO_5PS$
Molecular weight: *Acid* 169.07 g/mole; *IPA salt* 228.19 g/mole; *TMS salt* 245.23 g/mole
Description: *Acid* white solid, odorless; *TMS salt* Clear amber to yellow liquid; and slight sulfur odor as the 70% aqueous technical (dry pure glyphosate TMS salt is strongly hygroscopic and difficult to maintain; thus, a 70% aqueous solution is used as the technical grade material)
Density: *Acid* 1.74 g/mL; *70% Aqueous TMS salt* 1.23-1.25 g/mL (20 C)
Melting point: 200 C (with decomposition)
Boiling point: *Acid* NA; *70 % Aqueous TMS salt* 109 C (2.13×10^4 Pa)
Vapor pressure: *Acid* 2.45×10^{-8} Pa (45 C); *70 % Aqueous TMS salt* 3.99×10^{-5} Pa (25 C)
Stability: *Acid* stable for 32 d (25 C) and pH 5, 7, or 9; *70 % Aqueous TMS salt* stable for 32 d (25 C) and pH 7 or 9
Solubility:

Acid
water 15,700 mg/L (pH 7, 25 C); 11,600 mg/L (pH 2.5, 25 C)
Isopropylamine salt
water 900,000 mg/L (pH 7, 25 C) (estimated) (ref. 10); 786,000 mg/L (pH 4.06, 25 C)
Trimethylsulfonium salt
water 4,300,000 mg/L (pH 7, 25 C)

pK_a: *Acid* 2.6, 5.6, and 10.3 (Acts as a weak acid)
K_{ow}: 0.0006-0.0017

HERBICIDAL USE

Glyphosate is non-selective, foliar-applied, and can be used as follows; preplant or PRE at 0.21-2.24 kg ae/ha to control emerged weeds at planting in certain annual crops planted using no till methods; POST at 0.84-4.2 kg ae/ha or at 0.5-5% v/v of a 360 g/L product in a spray-to-wet application for general vegetation control in many noncrop areas such as industrial sites; directed POST or for site preparation at up to 4.2 kg ae/ha in ornamentals and Christmas trees; directed POST at 0.84-4.2 kg ae/ha in tree and vine crops; preharvest at 0.84-4.2 kg ae/ha in cotton; preharvest at 0.21-0.84 kg ae/ha in wheat; POST at 0.16 kg ae/ha in bahiagrass and Kentucky bluegrass, POST at 0.16-0.42 kg ae/ha in bermudagrass and POST at 0.21 kg ae/ha in fescues, orchardgrass, and quackgrass for suppression of these perennial grasses on orchard floors; and for control of woody vegetation by injection or frill treatment or by treating cut stumps. Glyphosate can be applied with a conventional sprayer, or with recirculating sprayers, shielded applicators, and wiper applicators. It controls virtually all annual and perennial weeds, but generally is most phytotoxic to annual grasses. A non-ionic surfactant is required for maximum efficacy, although certain formulated products already contain surfactant. In addition, selected formulations can be used POST in genetically modified crops tolerant to glyphosate (see mechanism of resistance section) such as soybean, corn, cotton, and canola.

USE PRECAUTIONS

Fire hazard: All aqueous products (ROUNDUP, RODEO, etc.) are non-flammable; flash point is >93 C.
Corrosiveness: Corrosive to iron and galvanized steel; do not hold spray mixture in galvanized or unlined steel tanks (except stainless) for extended periods.
Storage stability: All products containing only glyphosate isopropylamine salt are stable at <60 C; they freeze at -29 C but can be used upon thawing. Package mixtures may have

different characteristics.

Cleaning glassware/spray equipment: Clean glassware with water. Flush sprayer parts with several changes of water.

Emergency exposure: Glyphosate is a potential irritant. No specific antidote is available. Flush eyes with water for at least 15 min. If ingested, immediately dilute by swallowing milk or water.

Incompatibilities: Tank mixing with residual herbicides such as substituted ureas and triazines or with POST herbicides such as paraquat, dalapon, MSMA, phenoxy, or other auxin type herbicides may reduce glyphosate efficacy.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits enolpyruvyl shikimate-3-phosphate (EPSP) synthase (more details on page 13)

Symptomology: Growth is inhibited soon after application followed by general foliar chlorosis and necrosis within 4-7 d for highly susceptible grasses and within 10-20 d for less susceptible species. Chlorosis may appear first and be most pronounced in immature leaves and growing points. Foliage sometimes turns reddish-purple in certain species Regrowth of treated perennial and woody species often appears deformed with whitish markings or striations; multiple shoots (sometimes called a witch's broom) may develop at the nodes.

Absorption: Moderately absorbed across the cuticle when POST applied (3, 13). The isopropylamine salt of glyphosate is more readily absorbed than is glyphosate acid, and surfactant and ammonium sulfate further increase absorption of the isopropylamine salt (12). Glyphosate transport across the plasmalemma is slower than most herbicides (especially non-polar herbicides) (9), probably because of its negative charge at physiological pH. A phosphate transporter may contribute to glyphosate movement across the plasmalemma (5).

Translocation: Primarily translocated in the symplast with accumulation in underground tissues, immature leaves, and meristems (14). Apoplastic translocation has been observed in tall morningglory (6) and quackgrass (10), but most results suggest little to no apoplastic movement. Glyphosate may interfere with its own translocation from treated leaves by interfering with carbon partitioning and metabolism (8).

Metabolism in plants: Not appreciably metabolized when applied at phytotoxic rates. Glyphosate is slowly metabolized to amino methylphosphonic acid (AMPA) (4, 15).

Non-herbicidal biological properties: Sublethal rates inhibit seedhead emergence and suppress vegetative growth of most perennial grasses.

Mechanism of resistance in weeds: Three mechanisms of resistancehave been identified. 1) Altered uptake and translocaiton; 2) Taget site mutation; and 3) Amplificaiton of the EPSPS gene.

Engineered tolerance in crops: Available in several species, including tobacco, tomato, petunia, corn, chicory, cotton, canola, carrot, and soybean. *Corydalis*, and certain bacteria species.

BEHAVIOR IN SOIL

Sorption: Rapidly and tightly absorbed to soil. OM, clay, silt, or sand content and soil pH have minimal effect on adsorption. Glyphosate adsorption correlates with the amount of vacant phosphate sorption sites and may occur through binding of the phosphonic acid moiety. High levels of metallic cations in clay soils increase the amount of glyphosate adsorbed. Strong adsorption to soils is evidenced in part by low phytotoxicity with soil applications. Crops can be seeded or transplanted immediately into treated areas.

K_{oc}: Average is 24,000 mL/g (estimated) (16)

K_d: 324-600 mL/g for a silty clay loam and a loamy sand

Transformation:

Photodegradation: Negligible losses

Other degradation: Degraded microbially in soil and water. Decomposition rates vary with soil and microbial population. From 10 to 70% of glyphosate may be transformed to CO_2 over a growing season or less. Non-microbial degradation rates are negligible.

Persistence: Glyphosate has moderate persistence with a typical field half-life of 47 d (16). All crops can be planted immediately after application due to strong adsorption to soil.

Lab experiments: Half-life typically is <25 d

Mobility: Low mobility on most soils in field and lab studies because of strong adsorption to soil; low potential for movement in runoff in field and lab studies

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade glyphosate acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 5600 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Glyphosate isopropylamine salt technical: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Glyphosate trimethysulfonium salt technical: Oral LD_{50} male rat, 748 mg/kg; female Glyphosate at, 755 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} >5.18 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, mild; Eye irritation rabbit, mild

ROUNDUP: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, 3.2 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

LANDMASTER BW: Oral LD_{50} rat, 3860 mg/kg; Dermal LD_{50} rabbit, 6366 mg/kg; Skin irritation rabbit, moderate; Eye irritation rabbit, severe

Subchronic toxicity:

90-d dietary, mouse: NOEL 2300 mg/kg/d (10,000 mg/kg); decreased weight gains at 50,000 mg/kg

90-d dietary, rat: NOEL >1400 mg/kg/d (20,000 mg/kg)

21-d dermal, rabbit: Systemic NOEL >5000 mg/kg/d; slight irritation at site of application at 5000 mg/kg/d

Chronic toxicity:

24-mo dietary, mouse: Oncogenic NOEL 4500 mg/kg/d (30,000 mg/kg); slightly lower body weight gains and several microscopic liver changes at 4500 mg/kg/d; not carcinogenic

24-mo dietary rat: NOEL 400 mg/kg/d (8000 mg/kg) carcinogenic; reduced body weight gains in females and eye changes at 1000 mg/kg/d (20,000 mg/kg)

12-mo dietary, dog: NOEL 500 mg/kg/d; no effects

Teratogenicity:

Rat: NOEL 1000 mg/kg/d; maternal and fetal mortality at 3500 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 175 mg/kg/d; fetal >350 mg/kg/d; maternal toxicity at 350 mg/kg/d; no fetal toxicity

Reproduction:

Rat: NOEL ~700 mg/kg/d (10,000 mg/kg); not reproductive toxin; decreased adult and pup body weight gains and possible changes in litter size at ~2100 mg/kg/d (30,000 mg/kg)

Mutagenicity:

Gene mutation: Ames test, negative; *E. coli,* negative; *B. subtilis* rec+ and rec-, negative; CHO/point mutation, negative

Structural chromosome aberration: Mouse dominant lethal, negative; Rat bone marrow/cell clastogensis, negative

DNA damage/repair: Rat primary culture/DNA repair, negative

Wildlife:

Bobwhite quail oral LD$_{50}$, >4640 mg/kg; 8-d dietary LC$_{50}$, >4640 mg/kg; Mallard duck 8-d dietary LC$_{50}$, 4640 mg/kg; Honey bee, oral LD$_{50}$, >100 ∝g/bee; topical LD$_{50}$, >100 μg/bee; Daphnia 48-h LC$_{50}$, 780 mg/L; Bluegill sunfish 96-h LC$_{50}$, 120 mg/L; Harlequin fish 96-h LC$_{50}$, 168 mg/L; Rainbow trout 96-h LC$_{50}$, 86 mg/L; Atlantic oyster 96-h LC$_{50}$, >10 mg/L; Fiddler crab 96-h LC$_{50}$, mg/L; Shrimp 96-h LC$_{50}$, 281 mg/L

Glyphosate trimethylsulfonium salt technical: Bobwhite quail 8-d dietary LC$_{50}$, >5000 mg/kg; Mallard duck oral LD$_{50}$, 950 mg/kg; 8-d dietary LC$_{50}$, >5000 mg/kg; Honey bee topical LD$_{50}$, >62.1 μg/bee; Daphnia 48-h LC$_{50}$, 71 mg/L; Bluegill sunfish 96-h LC$_{50}$, 3500 mg/L; Rainbow trout 96-h LC$_{50}$,1800 mg/L; Mysid shrimp 96-h LC$_{50}$, 17.4 mg/L

ROUNDUP: Earthworm LC$_{50}$ in soil, >5000 mg/kg; Honey bee, oral LD$_{50}$, >100 μg/bee, topical LD$_{50}$, >100 μg/bee; Daphnia 48-h LC$_{50}$, 5.3-37 mg/L; Bluegill sunfish 96-h LC$_{50}$, 5.8-14 mg/L; Carp 96-h LC$_{50}$, 19.7 mg/L; Catfish 96-h LC$_{50}$, 16 mg/L;

trout 96-h LC$_{50}$, 8.2-26 mg/L; Crayfish 96-h LC$_{50}$, >1000 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Recrystallize three times from water

Analytical methods: Assay method for formulated product uses HPLC. Separation is obtained using a strong anion exchange column and a phosphate buffered mobile phase. AOAC Official Method is 983.10.

Historical: Herbicidal activity was first reported in 1971 (2). Glyphosate-isopropylammonium salt and glyphosate-sesquisodium salt were introduced by Monsanto Company. The trimethylsulfonium salt was introduced in Spain in 1989 by ICI Agrochemicals U.S. patent 3,799,758 was awarded to Monsanto. European patent 53,871 and U.S. patent 4,315,765 both were awarded to ICI.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Adama; BASF; Cheminova; Dow AgroSciences; Drexel; Helena; Monsanto; Syngenta Crop Protection

Reference(s):

1. Amrhein, N. et al. 1980. Plant Physiol. 66:830.
2. Baird, D. D. et al. 1971. Proc. North Cent. Weed Control Conf. 26:64.
3. Boerboom and Wyse. 1988. Weed Sci. 36:291.4. Coupland, D. 1984. Pestic. Sci. 15:226.
5. Denis and Delrot. 1993. Physiol. Plant. 87:569.
6. Dewey and Appleby. 1983. Weed Sci. 31:308.
7. Duke and Hoaglan. 1978. Plant Sci. Lett. 11:185.
8. Geiger and Bestman. 1990. Weed Sci. 38:324.
9. Jachetta, J.J. et al. 1986. Plant Physiol. 82:1000.
10. Klevon and Wyse. 1984. Weed Sci. 32:744.
11. Lee, T. T. 1980. Weed Res. 20:365.
12. MacIssac, S. A. et al. 1991. Pestic. Sci. 31:53.
13. Marshall, G. et al. 1987. Pestic. Sci. 18:55.
14. Martin and Edgington. 1981. Pestic. Biochem. Physiol. 16:87.
15. Sandberg, C. L. et al. 1980. Weed Res. 20:195.
16. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

halauxifen methyl

Cas #: 943831-98-9 $4^{(O)}$

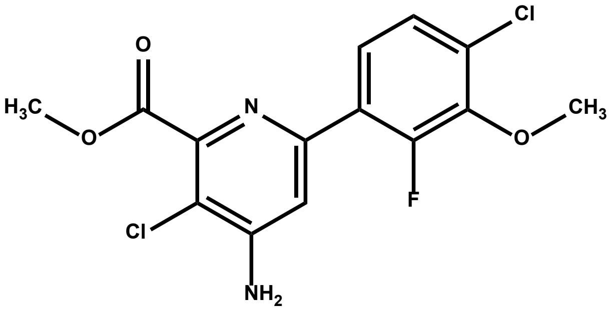
methyl 4-amino-3-chloro-6-(4-chloro-2-fluoro-3-methoxyphenyl)-2-pyridinecarboxylate

NOMENCLATURE

Common name: halauxifen methyl (ISO provisionally approved in 2012)
Other name(s): methyl 4-amino-3-chloro-6-(4-chloro-2-fluoro-3-methoxyphenyl)picolinate (IUPAC)
Tradename(s): Arylex$^{\text{TM}}$ Active herbicide, Pixarro$^{\text{TM}}$ herbicide, Paradigm$^{\text{TM}}$ herbicide.
Chemical family: arylpicolinate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
Herbicide



Molecular formula: $C_{14}H_{11}Cl_2FN_2O_3$
Molecular weight: 345.17 g/mole
Description: Off white powder
Density: 1.5057 g/cm^3
Melting point: 145.5 C
Boiling point: Decomposes before boiling
Vapor pressure: 5.9 x 10^{-9} Pa (20 C)
Stability: Aqueous Photostability (DT_{50}): pH 4 = 81 days; pH 7 = 155 days; pH 9 = 3 days
Solubility: g/l @ 20 C

- Water
  - pH 5: 1.66 mg/L
  - pH 7: 1.67 mg/L
  - pH 9: 1.69 mg/L
- Acetone: >250 g/L
- Ethyl Acetate: 114 g/L
- 1,2-Dichloroethane: 54.3 g/L
- Methanol: 31.7 g/L
- Octanol: 8.90 g/L
- Xylene: 8.24 g/L
- Heptane: 0.0375 g/L

pK_a: 2.84 at 20 C
K_{ow}: log K_{ow} = 3.76

HERBICIDAL USE

Selective postemergence broadleaf weed control in cereals and other crops.

USE PRECAUTIONS

Fire hazard: AI is not highly flammable
Corrosiveness: not available
Storage stability: not available
Cleaning glassware/spray equipment: not available
Emergency exposure: AI is not explosive.
Incompatibilities: none known

BEHAVIOR IN PLANTS

Mechanism of action: Synthetic auxin (HRAC group O, WSSA group 4) (more details on page 12)
Symptomology: Cessation of growth, stem and petiole epinasty, and leaf malformations are typical.
Absorption/translocation: Readily absorbed through leaves, shoots and roots. Systemically mobile in phloem and xylem.
Metabolism in plants: De-esterified to the active mobile form, halauxifen-acid, in all plants. O-demethylation on the aryl ring occurs followed by glucose conjugation leading to further more complex conjugates. Relative rate of these two processes likely influences the degree of plant species susceptibility. Halauxifen-acid degradation in cereals is rapid, limiting the accumulation of active herbicide residues in straw.
Non-herbicidal biological properties: None known.
Mechanism of resistance in weeds: None known.

BEHAVIOR IN SOIL

Sorption: Kd 13 -340 mL/g (average = 73 mL/g)
Koc 473 – 2659 mL/g (average = 1418 mL/g)
Transformation:
Photodegradation: Aqueous DT50 = 0.129 hours at pH 7. Insignificant on soil.
Other degradation: Hydrolyzes to halauxifen-acid as primary metabolite
Persistence: Average laboratory DT50: halauxifen-methyl = 1.5 days, halauxifen-acid = 14 days.
Field experiments: Field dissipation studies following spring applications at 6 sites in North America resulted in an average half-life of 15 days for halauxifen methyl. Field dissipation studies following spring or autumn applications at 4 sites in Europe resulted in an average half-life of 17 days for halauxifen methyl.
Mobility: Field dissipation studies showed limited movement of halauxifen-methyl or halauxifen acid with residues mainly detected in the top 15 cm of the soil profile.
Volatilization: Insignificant

TOXICOLOGICAL PROPERTIES

A complete set of mammalian toxicology studies was conducted with halauxifen-acid (halauxifen) and an extensive set of additional toxicity studies was conducted with halauxifen methyl in order to provide comparative information. The acute mammalian toxicity of halauxifen-acid and halauxifen methyl are low by the oral and dermal routes of exposure. The compounds are minimally irritating to the eyes and skin and are not dermal sensitizers. Long-term toxicity and carcinogenicity studies with

halauxifen-acid in rats and mice did not demonstrate any potential for carcinogenicity. The results of

these studies are summarized in the following table.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal rabbit LD_{50}, >5000 mg/kg;; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

1 lb/gal formulation: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL 250 mg/kg/d (HDT)

Chronic toxicity:

18-mo dietary, mouse: NOEL 100 mg/kg/d (HDT); not carcinogenic

Teratogenicity:

Mice: NOEL 50 mg/kg/d

Reproduction:

Rat: NOEL 450 mg/kg/d (HDT)

Mutagenicity:

Ames Test: negative

Wildlife:

Testing of halauxifen methyl indicates that it exhibits very low acute toxicity to terrestrial species: birds, honeybees and earthworms. Halauxifen methyl exhibits moderate acute toxicity to fish and aquatic invertebrates, and moderate to high toxicity to freshwater and marine algae depending upon species.

Avian oral: Bobwhite Quail LD_{50} >2250 mg/kg bw; Avian dietary Bobwhite Quail LC_{50} >5620 mg/kg diet; Avian dietary Mallard duck LC_{50} >5620 mg/kg diet; Fish acute: Rainbow trout LC_{50} = 2.01 mg/L (96 hr) Invertebrate acute: Water flea EC_{50} = 2.12 mg/L (48hr); Freshwater Algae: Green alga EC_{50} > 0.245 mg/L (96 hr); Freshwater Algae: Diatom EC_{50} = 0.663 mg/L (96 hr); Freshwater Algae: Bluegreen alga EC_{50} > 0.775 mg/L (96 hr); Marine Algae: Diatom EC_{50} = 1.07 mg/L (96 hr); Honeybee, contact: Honeybee LD_{50} >98.1 ug/bee, Honeybee, oral:Honeybee LD_{50} >108 ug/bee; Earthworm, acute (14d): Compost worm LC_{50} >1000 mg/kg soil

Use classification: Caution

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Not available

Purification of technical: Not available

Analytical methods: Not available

Historical: Discovered by Dow AgroSciences in 2005.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

halosulfuron-methyl

CAS #: 100784-20-1

2$^{(B)}$

methyl 3-chloro-5-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino] carbonyl]amino] sulfonyl]-1-methyl-1*H*-pyrazole-4-carboxylate

NOMENCLATURE

Common name: halosulfuron-methyl

Other name(s): halosulfuron-methyl (ISO 1750 published); MON 12000; MON 12037; NC-319; methyl 3-chloro-5-(4,6-dimethoxypyrimidin-2-ylcarbamorylsulfamoyl)-1-1-methylpyraxole-4-carboxylate (IUPAC)

Trade name(s): PERMIT®; SANDEA®; SEMPRA®; YUKON™; PERMIT PLUS®; SEDGEHAMMER®; SEDGEHAMMER PLUS®

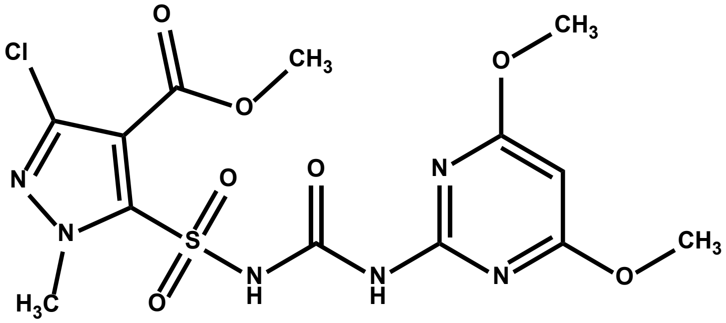
Chemical family:

pyrazole; pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

halosulfuron



Molecular formula: $C_{13}H_{15}ClN_6O_7S$

Molecular weight: 434.81 g/mole

Description: White powder

Density: 1.62 g/mL (25˚C)

Melting point: 175.5-177.2˚C

Boiling point: NA

Vapor pressure: $<1 \times 10^{-5}$ Pa

Stability: Stable except at high humidity

Solubility:

Water, 15 mg/L (pH 5, 25 C); 1630 mg/L (pH 7, 20 C)

pK$_a$: 3.5 (weak acid)

K$_{ow}$: 47 (pH 5, 20˚C); 0.96 (pH 7, 20˚C); 0.29 (pH 9, 20˚C)

HERBICIDAL USE

Halosulfuron can be applied early preplant surface, PPI, or PRE to corn at 73-84 g ai/ha, POST in corn and grain sorghum at 36 g ai/ha, POST in warm and cool season turfgrass at 35-70 g ai/ha, and POST in sugarcane at 18-140 g ai/ha. Other crops include rice, asparagus, cucurbits, dry beans, succulent snap beans, fruiting vegetables, apples, rhubarb, bushberries, okra, tree nuts, cotton and alfalfa. Weeds controlled included velvetleaf, cocklebur, and numerous other broadleaf weeds, as well as *Cyperus* species (nutsedge).

USE PRECAUTIONS

Fire hazard: Technical and formulated products are dry and non-flammable.

Corrosiveness: Technical and formulated products are non-corrosive.

Storage stability: Technical and formulated products are stable unless exposed to high humidity.

Emergency exposure: Wash eyes with clean water for 15-20 min. and get medical attention. Wash skin with soap and water.

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Rapid growth inhibition with POST application. Chlorosis occurs within 3-7 d after application, appearing faster under good growing conditions. Death of the growing point occurs within 7-14 d, although complete death may require 14-21 d. PRE application does not inhibit seed germination. The shoot growing point becomes chlorotic and necrotic soon after seedling emergence. Cotyledons of some species such as cocklebur can remain green for nearly 2 wk before dying.

Absorption/translocation: Root absorption in hydroponics is faster at lower pH. Approximately 10-11% of halosulfuron-methyl supplied to corn roots is absorbed at pH 4 in 24 h, whereas 5-7% is absorbed at pH 7. Corn leaves absorbed 7-9% of applied halosulfuron after 4 h while velvetleaf leaves absorbed 20-25%. Less than 14% of applied halosulfuron translocates in corn.

Metabolism in plants: PRE applications of halosulfuron result in rapid soil degradation followed by uptake of the resulting pyrazole metabolite (residues are almost exclusively derived from the pyrazole ring). Little halosulfuron is metabolized in corn, sugarcane, soybean, and wheat following foliar application.

Non-herbicidal biological properties: NA

Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: Moderately absorbed in soil

K$_{oc}$, K$_d$, K$_f$: K$_{oc}$ 93.5 mL/g, K$_d$ 1.66 mL/g, K$_f$ 1.48 mL/g, 0.76 mL/g for a Drummer silty clay loam; K$_{oc}$ 113.7 mL/g, K$_d$ 0.66 mL/g, K$_f$ 0.68 mL/g for Sarpy soil; K$_{oc}$ 199.2 mL/g, K$_d$ 3.98 mL/g, K$_f$ 3.56 mL/g for a Sable soil; K$_{oc}$ 31.1 mL/g, K$_d$ 0.36 mL/g, K$_f$ 0.32 mL/g for a Spinks soil

Transformation:

Photodegradation: Negligible losses

Other degradation: Degraded by microbes and by non-microbial hydrolysis with rapid rates in both high and low pH soils. Under anaerobic conditions, however, microbial degradation is slow and most degradation is by hydrolysis. The major metabolites under acidic conditions are 3-chlorosulfonamide acid and aminopyrimidine resulting from 5sulfonylurea bridge hydrolysis. Major metabolite in basic soils is a rearrangement ester of the parent halosulfuron. Halosulfuron eventually degrades to CO_2.

Persistence: Short to moderate persistence

Field experiments: Half-lives as follows: 4-12 d in a Norfolk sandy loam in North Carolina with 1% OM, pH 6.0, and 246 cm of rainfall received during the study; 34 d in Harpster loam in Illinois with 4.8% OM, pH 7.7, and 178 cm of rainfall; 18 d in a Harp loam in Iowa with 4.5% OM, pH 6.5, and 185 cm of rainfall; 6 d in Uvalde clay in Texas with 2.1% OM, pH 8.3, and 147 cm of rainfall.

Lab experiments: Half-lives as follows: 9-14 d in an aerobic silty clay loam with 0.8% OM and pH8; 14-18 d in an aerobic sandy loam with 3.5% OM and pH 6; 19-27 d in an anaerobic (aquatic) clay loam with pH 7.

Mobility: Halosulfuron has low to moderate leaching potential. GUS index score (1) was 2.41 and median leaching concentration was 0.03 ug/L when application rate was 0.23 lb/A, half-life was 26 d, K_{oc} was 199 mL/g, and pH was 6; GUS index score was 1.76 and median leaching concentration was 3 x 10^{-3} ug/L when application rate was 258 g/ha half-life was 8 d, K_{oc} was 113 mL/g, and pH was 8.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 8866 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 0.006 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, mouse: In Study, NOEL 6400 mg/kg; no effects. In Study 2, NOEL 3500 mg/kg; decreased body weight gain and white cell counts, increased hemoglobin and liver weights, and possible histopathological changes of the thymus at 7000 mg/kg

90-d dietary, rat: NOEL 0.2 mg/kg/d; decreased body weight gain, slight changes in clinical chemistry parameters, and minor histopathological changes in the kidney and liver at 6400 mg/kg; equivocal effects at 1600 mg/kg

90-d dietary, dog: NOEL NA; decreased body weight gain, decreased cholesterol, increased liver weights, slight anemia in females, and decreased white blood cells in males at 160 mg/kg/d; decreased body weight gains in females and lower cholesterol levels in males at 40 mg/kg/d; equivocal decrease in weight gain at 10 mg/kg/d

21-d dermal study, rat: NOEL >1000 mg/kg/d; no effects

Chronic toxicity:

18-mo dietary, mouse: NOEL male 410 mg/kg/d; female >1200 mg/kg/d; equivocal epididymal lesion at 1200 mg/kg/d; not carcinogenic

24-mo dietary, rat: NOEL 56 mg/kg/d; reduced body weight gains at 2500 mg/kg; not carcinogenic

12-mo dietary, dog: NOEL male 1 mg/kg/d, femail 10 mg/kg/d; decreased body weight gains, cholesterol levels, and lymphocyte values in males, and decreased red cell parameters in females at 40 mg/kg/d; decreased body weight gains and cholesterol levels in males at 10 mg/kg/d

Teratogenicity:

Rat: NOEL 250 mg/kg/d; clinical signs of toxicity, decreased maternal weight gain, increased post-implantation loss, decreased fetal weights and increased incidence of malformations/variations at 750 mg/kg/d

Rabbit: NOEL 50 mg/kg/d; reduced maternal body weight gain and increased post-implantation loss at 150 mg/kg/d

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 5-d dietary LC_{50}, >5620 mg/kg, 1-generation reproduction NOEC, 1000 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg, 1-generation reproduction NOEC, 1000 mg/kg; Honey bee topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >107 mg/L; Bluegill sunfish 96-h LC_{50}, >118 mg/L; Rainbow trout 96-h LC_{50}, >131 mg/L; Sheepshead minnow 96-h LC_{50}, >125 mg/L; Mysid shrimp 96-h LC_{50}, 109 mg/L; Oyster 96-h shell deposition EC_{50}, 94 mg/L; Selenastrum ED_{50}, 0.0053 mg/L

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: Mouse micronucleus, negative; *In vitro* cytogenetics, negative

DNA damage/repair: Rat hepatocyte/UDS, negative

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Synthesized and discovered by Nissan Chemical Industries, Ltd. of Tokyo, Japan; introduced at the Brighton Centre Nov. 19, 1991; commercial products are being developed in the U.S. by Gowan Company.

MANUFACTURER(S) AND INFORMATION SOURCES:

Manufacturer(s): Nissan Chemical Industries

Source(s): Gowan Company

Reference(s):

1. Gustafson, D.I. 1989, Environ. Toxicol. Chem. 8:339.
2. LaRossa and Schloss. 1984. J. Biol. Chem. 259:8753.

haloxyfop

2-[4-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy] propanoic acid

CAS # Acid (R,S): 69806-34-4
Acid (R isomer): 95977-29-0
Ethoxyethyl ester: 87237-48-7
Methyl ester: 69806-40-2

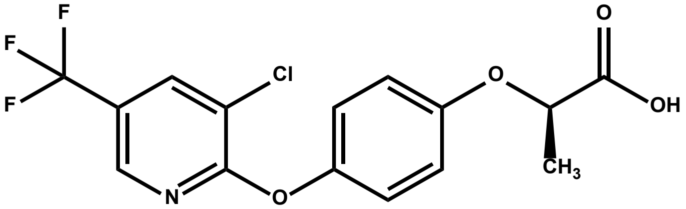
1$^{(A)}$

NOMENCLATURE

Common name: haloxyfop (ANSI, ISO, WSSA) for the racemic mixture of R and S isomers; haloxyfop-P for the R isomer.
Other name(s): DOWCO 453 ME; (Acid) (RS)-2-[4-(3-chloro-5-trifluoromethyl-2-pyridyloxy)phenoxy] propionic acid (IUPAC); haloxyfop-P=(R)-2-{4-[3-chloro-5-trifluoromethyl-2-pyridyloxy]phenoxy} propionic acid (IUPAC); (Methyl ester) haloxyfop-methyl=methyl (RS) 2-{4-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy}propionate (IUPAC); haloxyfop-P methyl = methyl (R) 2-{4-[3-chloro-5-(trifluoromethyl)-2-pyridyloxy]phenoxy}propionate (IUPAC); not registered in U.S.
Trade name(s): GALENT™; VERDICT™; ZELLECK™; FOCUS®
Chemical family: aryloxyphenoxy propionate; aryloxyphenoxy propionic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
haloxyfop (R,isomer)



Molecular formula: Acid $C_{15}H_{11}ClF_3NO_4$; Ethoxyethyl ester $C_{19}H_{19}ClF_3NO_5$; Methyl ester $C_{16}H_{13}ClF_3NO_4$
Molecular weight: Acid 361.70 g/mole Ethoxyethyl ester 433.70 g/mole; Methyl ester 375.50 g/mole
Description: Acid White crystal, offensive odor; Ethoxyethyl ester Yellow-orange solid, mild aromatic odor; Methyl ester Amber to straw yellow solid, mild aromatic odor
Density: Ethoxyethyl ester 0.978 g/mL; Methyl ester 0.968 g/mL
Melting point: Acid 107-108 C; Ethoxyethyl ester 56-58 C; Methyl ester 55-57 C
Boiling point: NA
Vapor pressure: Acid $<1.7 \times 10^{-5}$ Pa (25 C); Ethoxyethyl ester 4.5×10^{-4} Pa (25 C); Methyl ester 8.67×10^{-5} Pa (25 C)
Stability: Methyl ester stable to UV light; No decomposition after 88 h at 200 C
Solubility:

Acid
water 43.3 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C)
acetone >100 (20 C)   methanol >100 (20 C)
dichloromethane 45.9   Propan-2-ol >100 (20 C)
ethyl acetate 51.8   toluene 11.8
n-hexane 0.017   xylene 7.4 (20 C)

Ethoxyethyl ester
water 0.58 mg/L (20 C)
organic solvents g/100 mL (25 C)
acetone >100   methylene chloride 276
dichloromethane >100   Propan-2-ol 5.2
ethyl acetate >100   toluene >100
n-hexane 4.4   xylene 125
methanol 23.3

Methyl ester
water 9.3 mg/L (25 C)
organic solvents g/100 mL (20 C)
acetone 335   methylene chloride 300
acetonitrile 400   xylene 127
isopar M 1.3

pK_a: 4.33 (weak acid)
K_{ow}: Acid 22 (20 C); Ethoxyethyl ester 21,600; Methyl ester 11,700

HERBICIDAL USE

Haloxyfop can be applied POST at 0.14-0.6 kg ai/ha in cotton, soybeans, sunflowers, sugarbeets, oilseed rape, potatoes, field beans, peas, flax, oil palm, peanuts, vine crops, and certain other minor crops. It controls annual and perennial grass with the higher rate needed for perennials. Major susceptible species include foxtail spp., barnyardgrass, crabgrass spp., Panicum spp., Brachiaria spp., bluegrass spp., goosegrass, blackgrass, wild oats, quackgrass, shattercane, johnsongrass, bermudagrass, woolly cupgrass, sprangletop, and Lolium spp. Rate of haloxyfop-P are about one-half those of haloxyfop. A surfactant or oil adjuvant is required for maximum efficacy, although certain commercial formulations already contain sufficient adjuvant.

USE PRECAUTIONS

Fire hazard: Technical is non-flammable. The product VERDICT is non-flammable; flash point is 43 C. The products GALLANT and ZELLECK are non-flammable; flash points are 47 C.
Corrosiveness: Non-corrosive (Acid)
Storage stability: Acid Stable for > 6 mo at 38 C; Formulated products have > 2 yr shelf life at room temperature
Cleaning glassware/spray equipment: Rinse equipment with soap and water
Emergency exposure: Wash skin with soap and water. Flush eyes with water for at least 5 min; get medical attention if irritation persists. If ingested, drink 1-2 glasses of water and induce vomiting; call a physician.
Incompatibilities: Haloxyfop can be antagonized by certain herbicides, especially those that produce rapid leaf necrosis.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)

Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop within 1-3 wk of application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.

Absorption: The haloxyfop methyl ester is absorbed rapidly into leaves and is rainfast within about 2 h of (1). Haloxyfop ester readily diffuses across the plasmalemma. Once inside the cell, the ester is rapidly hydrolyzed to haloxyfop acid which remains dissociated in the relatively alkaline cytoplasm. Because of this low lipophilicity, the polar haloxyfop anion is largely prevented from diffusing back out across the plasmalemma. Haloxyfop methyl ester that is deesterified before entering the cell would tend to diffuse across the plasmalemma as the protonated haloxyfop acid (relatively lipophilic). Inside the cell haloxyfop acid dissociates to the anion, thereby trapping the herbicide in the phloem cells.

Translocation: Haloxyfop is principally translocated in the phloem cells. Foliar-applied haloxyfop accumulates in the meristematic regions. Translocation is low in some species but faster in others (2).

Metabolism in plants: Haloxyfop methyl ester is hydrolyzed rapidly in tolerant and susceptible plants to the herbicidally active haloxyfop acid. Five hours after corn leaves were treated with haloxyfop methyl ester, 50% of the applied was recovered as haloxyfop acid, 31% as unmetabolized haloxyfop methyl ester, and 19% as unidentified polar metabolites thought to be conjugated forms of the herbicide (4). Rates of deesterification and subsequent metabolism to polar products vary among grass species, and may account for differential susceptibility to the herbicide (2).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Haloxyfop resistance in biotypes of normally sensitive grass weeds, including Lolium multiforum (selected by diclofop use), has been associated with an insensitive ACCase. However, in diclofop-resistant rigid ryegrass (L. rigidum) from Australian, resistance to haloxyfop as well as cross-resistance to a number of other chemical families is not due to reduced ACCase sensitivity activity, but may be conferred by increased rates herbicide metabolism (5) or by sequestration away from the site of action.

BEHAVIOR IN SOIL

Transformation:

Soil: Haloxyfop methyl ester rapidly hydrolyzes to the acid form, haloxyfop, in moist soil. Further degradation produces the pyridinol, pyridinone and phenol metabolites under aerobic conditions. Less extensive degradation occurs under anaerobic conditions or via photodegradation, but the same metabolites are formed.

Aquatic systems: In sterile buffer, haloxyfop methyl ester is stable at pH4, but is similarly rapidly hydrolyzed to the acid form, haloxyfop at pH 7 and 9 which is then stable. In water/sediment systems, haloxyfop is also rapidly formed which degrades to give the pyridinol metabolite.

Soil persistence:

Field: When quantified as total haloxyfop (ester plus acid), the residue dissipates following spring application with a typical half-life of 2-3 weeks under various field conditions to give the pyridinol metabolite.

Lab: Under standard conditions, haloxyfop methyl ester rapidly degrades with a half-life <1 day to give haloxyfop, which degrades with a typical half-life of 2-8 weeks (20°C and 40% of maximum water holding capacity).

Sorption:

Limited data available for the ester forms due to their rapid conversion in moist soil to haloxyfop. Haloxyfop is weakly absorbed to soil. Two metabolites (pyridinol and pyridinone) are similarly weakly adsorbed, whilst a third (phenol) is more strongly adsorbed.

K_{foc}: 27-86 mL/g at pH 4.7-7.8 and 0.4-5.0% org. C for sorption of haloxyfop. The pyridinol, pyridinone and phenol metabolites gave K_{foc} values of 20-38, 14-35 and 387-729 mL/g, respectively.

Mobility:

Haloxyfop has potential to be mobile under vulnerable conditions but this is mitigated by its relatively short half-life, whilst the methyl ester is estimated to be non-mobile. No residues of either haloxyfop or its three soil metabolites have been detected in the leachate from regulatory lysimeter studies under realistic worst case conditions, or below 20 cm depth in field dissipation studies.

Volatilization:

Based upon its low vapor pressure (5.5×10^{-5} Pa), negligible losses are expected from soil under typical use conditions and this was confirmed by the results of a wind tunnel experiment.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade haloxyfop acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 337 mg/kg, female rat 545 mg/kg; Dermal LD_{50} rabbit, > 5000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, none; Skin sensitization Guinea pig, no; Eye irritation rabbit moderate

haloxyfop ethoxyethyl ester technical: Oral LD_{50} rat, 518 mg/kg; Dermal LD_{50} rabbit, > 5000 mg/kg, rat >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

haloxyfop methyl ester technical: Oral LD_{50} male rat, 300 mg/kg; female rat, 623 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, mouse: NOEL 0.2 mg/kg/d; hepatocellular hypertrophy associated with peroxisome proliferation at 2 mg/kg/d

90-d dietary, rat: NOEL 0.2 mg/kg/d; hepatocellular hypertrophy associated with peroxisome proliferation and increased pigment in renal epithelial cells at 2 mg/kg/d

90-d dietary, dog: NOEL 2 mg/kg/d; hepatocellular hypertrophy associated with peroxisome proliferation, decreased serum cholesterol and red blood cell count at 20 mg/kg/d

90-d dietary, monkey: NOEL 2 mg/kg/d; hepatocellular hypertrophy associated with peroxisome proliferation decreased serum cholesterol and triglyceride at 30 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 0.065 mg/kg/d; increased eosinophilic staining of hepatocytes and increased hepatocellular carcinomas associated with peroxisome proliferation at 0.6 mg/kg/d

24-mo dietary, rat: NOEL 0.065 mg/kg/d; increased eosinophilic staining of hepatocytes and increased pigment in renal epithelium at 0.1 mg/kg/d

12-mo dietary, dog: NOEL 0.5 mg/kg/d; decreased serum cholesterol at 5 mg/kg/d

Teratogenicity:

Rat: NOEL 7.5 mg/kg/d; not teratogenic

Rabbit: NOEL 20 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 1 mg/kg/d; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: Mouse micronucleus, negative; Human lymphocyte/ cytogenetics, negative

DNA damage/repair: Rat hepatocyte/UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LD_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, 96.4 mg/L; bluegill sunfish 96-h LC_{50}, 548 mg/L; Rainbow trout 96-h LC_{50}, 800 mg/L; honeybee contact and oral > 100 µg/bee

haloxyfop ethoxyethyl ester technical: Bobwhite quail 8-d dietary LD_{50}, >5620 mg/L; Mallard duck oral LD_{50}, >2150 mg/L; 8-d dietary LC_{50}, >4321 mg/L; Rainbow trout 96-h LC_{50}, 1.18 mg/L

haloxyfop methyl ester technical: Bobwhite quail oral LD_{50}, 1159 mg/kg; 8-d dietary LD_{50}, >5620; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; honey bee oral LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 6.2 mg/L; Bluegill sunfish 96-h LC_{50}, 0.3 mg/L; rainbow trout 96-h LC_{50}, >50 mg/L; fathead minnow 96-h LC_{50}, 0.3 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: To produce haloxyfop methyl ester, the dianion form of hydroquinone is generated from hydroquinone plus two equivalents of a strong base such as sodium hydroxide in a polar aprotic solvent such as dimethylsulfoxide. The hydroquinone dianion salt is then reacted with 2,3-dichloro-5-(trifluoromethyl)pyridine at 80-90 C to give (3-chloro-5-(trifluromethyl)pyridinyl-2-oxyphenol, as the phenate salt. To the intermediate pyridinyloxyphenate at 25-30 C is added methyl 2-halopropionate to provide the product. U.S. patent 4,275,212 for the synthesis was issued in 1981.

Purification of technical: The methyl ester can be isolated by the addition of water to the reaction mixture, followed by extraction of the product into perchloroethylene. The perchloroethylene/product solution is then extracted with water to remove residual dimethylsulfoxide solvent and salts. Removal of the perchloroethylene by distillation under reduced pressure yields the methyl ester product. The methyl ester also can be isolated by a sequence involving vacuum distillation of the reaction mixture to remove the dimethylsulfoxide solvent, followed by filtration of the salts, and finally a high temperature, vacuum distillation of the product.

Analytical methods: Residues of haloxyfop and/or Haloxyfop methyl ester and their conjugates can be extracted from crop, animal tissue and soil with caustic methanol. The extract is acidified and diluted prior to the SPE clean-up. The eluate is evaporated to dryness and the residues are reconstituted in a solvent containing the stable isotope of haloxyfop as an internal standard followed by ESI HPLC-MS/MS analysis. Residues of haloxyfop and its metabolites are extracted from an acidified water sample and purified using a SPE cartridge. The eluate is diluted with water and is then analyzed by ESI HPLC/MS/MS. Contact Dow AgroSciences for the most recent methods for crop, anima, soil and water.

Historical: Haloxyfop was discovered in 1976 and patented June 28, 1988; U.S. patent 4,753,673 was awarded to The Dow Chemical Company. It was first marketed in Argentina in 1986 as GALLANT. Currently it is marketed in over 30 countries under trade names of VERDICT, GALLANT, FOCUS®, and others but is not marketed in the U.S.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

Reference(s):

1. Bryson, C.T. 1988. Weed Technol. 35:115.
2. Buhler, D.D. et al. 1985. Weed Sci. 33:291.
3. Burton, J. D. et al. 1989. Pestic. Biochem. Physiol. 34:76.
4. Harrison and Wax. 1986. Weed Sci. 34:185.
5. Powles, S. B. et al. 1990. Pages 394-406 in M.B. Green , H.M. LeBaron, and W. K. Moberg, eds., Managing Resistance to Agrochemicals. Am. Chem. Soc. Symp. Ser. 421, Washington DC.
6. Secor and Cseke. 1988 Plant Physiol. 86:10.
7. Stolenberg, D.E. et al. 1989. Weed Sci. 37:512.

hexazinone

CAS #: 51235-04-2

$5^{(C_1)}$

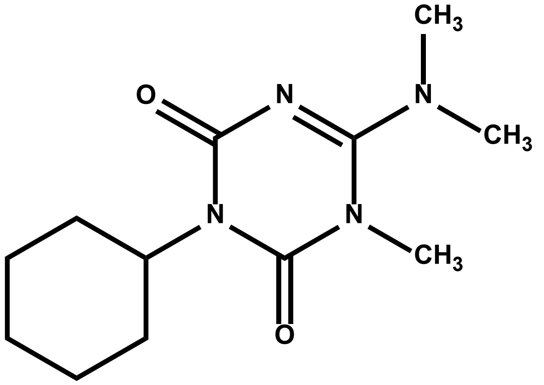
3-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1*H*,3*H*)-dione

NOMENCLATURE

Common name: hexazinone (ANSI, BSI, ISO, WSSA)
Other name(s): DPX-A3674; 3-cyclohexyl-6-dimethylamino-1-methyl-1,3,5-triazine-2,4(1*H*,3*H*)-dione (IUPAC)
Trade name(s): OUSTAR®; PRONONE®; VELPAR®; VELPAR® ALFAMAX; VELPAR® ALFAMAX GOLD; VELPAR® ALFAMAX MP; VELPAR® DF; VELPAR® K-4 MAX; VELPAR® L; VELPAR® ULW; WESTAR™
Chemical family: *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *hexazinone*



Molecular formula: $C_{12}H_{20}N_4O_2$
Molecular weight: 252.32 g/mole
Description: White crystalline solid, negligible odor
Density: 1.25 g/mL
Melting point: 115-117C
Boiling point: NA
Vapor pressure: 2.7 x 10^{-5} Pa (25 C) (extrapolated); 9 x 10^{-3} Pa (86 C)
Stability: Slowly degraded by UV light in water
Solubility:
water 33,000 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 62.6
benzene 82.6
chloroform 580
n-hexane 0.2
methanol 211
toluene 33.5
pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

Hexazinone can be applied as follows: at 0.62-1.87 kg ai/ha in dormant or semi-dormant alfalfa; at 0.31-2.5 kg ai/ha in pineapple; PRE at 0.62-5 kg ai/ha or POST at 0.62-1.24 kg ai/ha in sugarcane; at 1.24-1.87 kg ai/ha before bud break in first-year Christmas tree plantings (certain species) and 1.24-2.5 kg ai/ha in established plantings (use directed sprays if applied after bud break); at 2.5-7.5 kg ai/ha for site preparation in reforestation areas to be planted to various conifer species; at 1.24-5 kg ai/ha for conifer release; and at 2.5-15 kg ai/ha in non-crop land including industrial sites, railroads, rights-of-way, and storage areas. It controls many annual and perennial broadleaf and grass weeds, as well as many brush species. Hexazinone has both foliar and soil activity. A surfactant increases efficacy for foliar applications, but may cause undesirable levels of crop injury in some situations.

USE PRECAUTIONS

Fire hazard: The product VELPAR L is flammable. Other products are dry or aqueous and are non-flammable.
Corrosiveness: All products are non-corrosive
Storage stability: Stable under normal storage conditions for >2 yr. Store above 32 C in a dry place. Keep container closed.
Cleaning glassware/spray equipment: Clean glassware with detergent followed by an acetone rinse; flush tank, pump, hoses, and boom with water after removing nozzle tips and screens (clean these parts separately)
Emergency exposure: Flush skin and eyes with water; get medical attention if eye irritation persists; harmful if ingested
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Foliar chlorosis followed by necrosis
Absorption/translocation: Readily absorbed by roots and translocated upward in the xylem (6). Hexazinone also is absorbed by leaves when foliar-applied, but is poorly translocated to other plant parts. POST activity is enhanced by addition of a non-ionic surfactant.
Metabolism in plants: Hexazinone was converted to several hydroxylated and/or demethylated triazinone metabolites in *Pyrus melanocarpa* and *Rubus hispidus* following root or foliar uptake. Accumulation in *P. melanocarpa* of higher levels of the mono-demethylated metabolite (3-cyclohexyl-6-methylamino-1-methyl-1,3,5-triazine-2,4-dione) compared to *R. hispidus* may contribute to the greater tolerance in *P. malanocarpa* (5). Metabolism contributed to hexazinone selectivity in red and jack pine (9) and probably in loblolly pine (6). Sugarcane metabolites include a hydroxylated derivative, a hydroxylated-demethylated derivative, and a hydroxylated-deaminated derivative (7).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Multiple herbicide resistance in annual ryegrass included resistance to hexazinone (2)

BEHAVIOR IN SOIL

Sorption: Freundlich isotherm constants (K_f) on Fallsington sandy loam and Flanagan silt loam were, respectively, 0.2 (slope 0.95) and 1.0 (slope 1.05)

K_{oc}: Average is 54 mL/g (8)

Transformation:

Photodegradation: Photodegraded ~20% in 8 wk when dissolved in water under artificial sunlight. Hexazinone is stable in the dark for at least 5-8 wk in aqueous solutions of 5 and 5990 mg/L (representing dilute and spray-tank concentrations), buffered at pH values of 5, 7, and 9, and held at temperatures of 15, 25, and 37 C. In studies on thin soil surfaces, 60% of applied hexazinone (10 ppm) was degraded during a 6-wk exposure to UV light. Photodecomposition rate is about 3X faster when small amounts of inorganic salts are present and about 7X faster in natural river water or in distilled water containing a photoinitiator.

Other degradation: Microbial degradation contributes to decomposition in soil, and the triazine ring is broken to liberate CO_2. Lab studies (1) were conducted in the dark with ^{14}C-labeled hexazinone at 4 and 20 mg/kg in two soils. Evolved $^{14}CO_2$ accounted for 45-75% of the original ^{14}C after 90-d incubations.

Persistence: Moderately long residual with a typical field half-life of 90 d (8)

Field experiments: Half-life was ~1 mo in a Keyport silt loam in Delaware, ~2 mo in a Flanagan silt loam in Illinois, and ~6 mo in a Dundee silt loam in Mississippi

Lab experiments: Half-life of ~4-5 mo in both silt loam and sandy loam soils in the greenhouse

Mobility: Helling mobility class 4

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade hexazinone unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1690 mg/kg; male guinea pig, 860 mg/kg; Dermal LD_{50} rabbit, >6000 mg/kg; 1-h inhalation LC_{50} rat, >7.48 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, severe

Subchronic toxicity:

90-d dietary, rat: NOEL male 1000 mg/kg; body weight effects

2-wk dietary, rat: NOEL NA; no evidence of cumulative toxicity in males at 300 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 200 mg/kg; hepatocellular adenoma at ≥2500 mg/kg

24-mo dietary, rat: NOEL 200 mg/kg; not oncogenic; body weight effects

12-mo dietary, dog: NOEL 200 mg/kg; body weight gain at ≥1500 mg/kg

Teratogenicity:

Rat: NOEL 100 mg/kg/d; not teratogenic; maternal/ embryo toxicity at ≥400 mg/kg/d

Rabbit: NOEL 125 mg/kg/d (highest level tested); not teratogenic

Reproduction:

Rat: NOEL 200 mg/kg in a 2-generation study; body weight gain; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: *In vivo* cytogenetics, negative; *In vitro* cytogenetics, mutagenic and non-mutagenic in separate trials

Wildlife:

Bobwhite quail oral LD_{50}, 2258 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck 8-d dietary LC_{50}, >10,000 mg/kg; Honey bee non-toxic; Daphnia 48-h LC_{50}, 151 mg/L; Bluegill sunfish 96-h LC_{50}, 370-420 mg/L; Fathead minnow 96-h LC_{50}, 274 mg/L; Rainbow trout 96-h LC_{50}, 320-420 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: See U.S. patent 3,983,112.

Purification of technical: Recrystallize from hexane: toluene 60:40.

Analytical methods: See Holt, 1981 (4)

Historical: Biological properties were first described in 1975 (3). Covered by U.S. patents 3,902,887 and 3,983,116 issued to DuPont Company.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

1. Bartha and Pramer. 1965. Soil Sci. 100:68.
2. Burnet, M. W. M. et al. 1991. Pages 427-428 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Ltd., Oxford.
3. Hernandez, T. J. et al. 1975. Proc. South. Weed Sci. Soc. 28:247.
4. Holt, R. F. 1981. J. Agric. Food Chem. 29:165.
5. Jensen and Kimball. 1990. Weed Res. 30:35.
6. McNeil, W. K. et al. 1984. Weed Sci. 32:739.
7. Reiser, R. W. et al. 1983. Biomed. Mass Spectrom. 10:581.
8. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
9. Wood, J. E. et al. 1992. Pestic. Biochem. Physiol. 44:108.

imazamethabenz methyl

2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1H-imidazol-2-yl]-4(or 5) -methylbenzoic acid (3:2)

CAS # Acid: 100728-84-5
Methyl ester: 81405-85-8

2$^{(B)}$

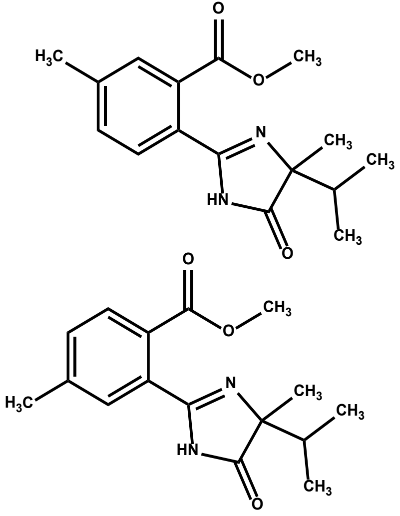
NOMENCLATURE

Common name: imazamethabenz (ANSI, BSI, ISO, WSSA); the commercial herbicide is a 3:2 mixture of the para- and meta-methyl isomers.
Other name(s): AC 222,293; reaction mixture of methyl 6-[(*RS*)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)-*m* toluate and methyl 2-[(*RS*)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)-*p* toluate (IUPAC)
Trade name(s): ASSERT®; AVERT®
Chemical family: imidazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure

Imazamethabemz methyl ester



Molecular formula: *Acid* $C_{15}H_{18}N_2O_3$; *Methyl ester* $C_{16}H_{20}N_2O_3$
Molecular weight: *Acid* 274.32 g/mole; *Methyl ester* 288.35 g/mole
Description: Off-white, fine to lumpy powder, slight musty odor
Density: 0.3 g/mL (20 C)
Melting point: 115-145 C (range due to isomer ratio)
Boiling point: NA
Vapor pressure: 1.5 x 10^{-6} Pa (25 C)
Stability: Stable after 24 mo (25 C); hydrolyzes rapidly in alkaline conditions, but slowly at pH 5 and 7. Stable in acidic conditions; rapidly degraded by UV light in aqueous solution; stable to heat decomposition temperature unknown
Solubility:
water (25 C), 1370 mg/L for the *m*-isomer, and 857 mg/L for the *p*-isomer
organic solvents g/100 mL (25 C) (isomeric mixture):
acetone 23
dichloromethane 30
DMSO 21.6
n-heptane 0.06
n-hexane 0-04
isopropanol18.3
methanol 30.9
methylene choloride 17.2
toluene 4.5
pK_a: 2.9 (23.5 C) (weak acid)
K_{ow}: NA

HERBICIDAL USE

Imazamethabenz can be applied POST at 0.35-0.53 kg ai/ha in wheat and barley, and POST at 0.2-0.43 kg ai/ha in sunflowers. It controls wild oats, roughstalk bluegrass, interrupted windgrass, wild mustard, London rocket, field pennycress, flixweed, tansymustard, catchweed, bedstraw, tartary buckwheat, and wild buckwheat. A non-ionic surfactant or oil adjuvant is required for maximum efficacy. Imazamethabenz can be applied in water or in non-phosphorus liquid fertilizer.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: The product ASSERT® is corrosive to carbon steel and aluminum; solvent may dissolve some plastics and nylon.
Storage stability: Shelf life is 2 yr
Cleaning glassware/spray equipment: Wash equipment with detergent. Wash glassware with detergent and rinse with methanol.
Emergency exposure: Causes irreversible eye damage. Wash skin with soap and water. If ingested, drink large quantities of milk, egg white, gelatin solution, or, if these are unavailable, water. Probable mucosal damage may contraindicate the use of gastric lavage.
Incompatibilities: ASSERT® is compatible with dicamba, or amine formulations of 2,4-D or MCPA. Alkaline products may cause imazamethabenz to precipitate from ASSERT® solutions. A white precipitate may form if ASSERT® is mixed in highly buffered alkaline water. Precipitate may form if ASSERT® is mixed with surfactants that contain buffering agents. If precipitation occurs, use sodium bisulfate to lower tank water pH.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth is inhibited within a few h after application, but injury symptoms usually do not appear for 1-2 wk or more. Meristematic areas become chlorotic, followed by slow general foliar chlorosis and necrosis.
Absorption/translocation: Rapidly and efficiently absorbed from root or shoot applications. Imazamethabenz methyl ester is highly xylem mobile. The herbicidally-active

deesterified imazamethabenz acid (but not the methyl ester) is mobile in the phloem. Imazamethabenz acid is produced in appreciable amounts only in susceptible weeds and accumulates in meristematic regions.

Metabolism in plants: Wheat tolerance is due to oxidation of the benzene methyl group to the corresponding hydroxymethyl derivative, followed by glucoside conjugation. Susceptible *Avena* spp. primarily deesterify imazamethabenz methyl ester, producing the phytotoxic imazamethabenz acid.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed in high pH soil, but adsorption increases with lower pH and higher clay and OM content. Sorption is reversible.

Transformation:

Photodegradation: Small losses can occur in the field. Half-life on soil is 30-60 d. Degradation by sunlight is rapid in water, however.

Other degradation: Primarily degraded by microbes. Non-microbial hydrolysis occurs more rapidly in high pH soils and produces the deesterified imazamethanbenz acid.

Persistence: Average half-life ranges from 25-36 d; planting of certain rotational crops may need to be delayed

Mobility: Field studies indicate that imazamethabenz remains in the top 45 cm of soil. Field studies suggest no potential for movement with surface water.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade imazamethabenz methyl ester unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 5.8 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

ASSERT 2.5 LC: Oral LD_{50} male rat, 2952 mg/kg, female rat, 3129 mg/kg; Dermal LD_{50} rabbit, >2171 mg/kg; 4-h inhalation LC_{50} rat, 5.6 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, corrosive

Subchronic toxicity:

90-d dietary, rat: NOEL 87.5 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL male 19.5; not oncogenic
24-mo dietary, rat: NOEL 12.5 mg/kg/d; not oncogenic
12-mo dietary, dog: NOEL 6.25 mg/kg/d

Teratogenicity: No teratogenic or fetotoxic effects

Rat: NOEL maternal < 250 mg/kg/d, fetal 250 mg/kg/d
Rabbit: NOEL maternal 750 mg/kg/d; fetal 250 mg/kg/d
Reproduction:Rat: NOEL 93.2 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative; CHO/ HGPRT, negative

Structural chromosome aberration: Rat dominant lethal, negative; CHO/CA, negative

DNA damage/repair: Primary rat hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg, 8-d dietary LC_{50}, >5000 mg/kg; Earthworm 14-d LC_{50} in soil, >123 mg/kg; Honey bee topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >100 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Imazamethabenz is extracted from grain with methanol in methylene chloride and from foliage with HCl in acetone: methanol. After removal of co-extractives by solvent partitioning, final clean-up is achieved on florisil. Residues are detected by GC methods with a nitrogen-phosphorus detector after derivatization or by HPLC. Validated sensitivity is 50 mg/kg.

Historical: Compound patent was received February 12, 1980 and the use patent on October 27, 1981. Herbicidal activity of imazamethabenz was first reported in 1982 (1, 2). An Experimental Use Permit in wheat and barley was granted in 1984. Section 18 Emergency Exemption was issued in 1986 for ASSERT use in sunflowers, and full registration was granted, April 11, 1988. Introduced by American Cyanamid Co. U.S. patents are 4,188,487 and 4,297,128.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Nufarm; Viterra

Reference(s):

1. Kirkland and Shafer. 1982. Proc. Brit. Crop Prot. Conf. Weeds 1:33
2. Shaner, D.L. et al. 1982. Proc. Brit. Crop Prot. Conf. Weeds. 1:25

imazamox

2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-5-(methoxymethyl)3-pyridinecarboxylic acid

CAS # Acid: 114311-32-9
NH_4 salt: 247057-22-3

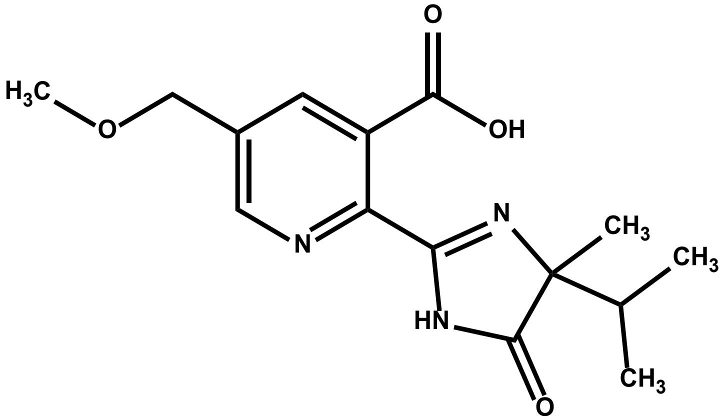
$2^{(B)}$

NOMENCLATURE

Common name: imazamox (ANSI, BSI, ISO, WSSA)
Other name(s): AC 299,263; 2-[(*RS*)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]-5-methoxymethylnicotinic acid (IUPAC)
Trade name(s): ABSOLUTE®; ADRENALIN® SC; ALTITUDE FX®; ARES™; BEYOND®; CLEARCAST®; CLEARMAX™; ODESSEY®; ODYSSEY DLX; RAPTOR®; VIPER® ADV
Chemical family: imidazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
imazamox acid



Molecular formula: *Acid* $C_{15}H_{19}N_3O_4$; *NH_4 salt* $C_{15}H_{22}N_4O_3$
Molecular weight: *Acid* 305.33 g/mole; *NH_4 salt* 322.36 g/mole
Description: Odorless, powdered solid
Density: 1.39 g/mL (20 C)
Melting point: 166.0-166.7 C (technical)
Boiling point: NA
Vapor pressure: 1.3×10^{-5} Pa (60 C)
Stability: Stable for >12 mo (37 C)
Solubility:
water miscible
organic solvents g/100 mL (20 C)
n-hexane 0.0006
toluene 0.21
dichloromethane 14.3
methanol 6.68
acetone 2.93
acetonitrile 1.85
ethyl acetate 1.02
pK_a: 2.3, 3.3, and 10.8; active ingredient will exist primarily in the singly ionized form in the pH range of 5-9.
K_{ow}: 5.36

HERBICIDAL USE

Imazamox is used POST at 20-53 g ae/ha depending on crop types in alfalfa, edible legumes, soybean and certain imidazolinone-tolerant crops such as Clearfield® canola, Clearfield® rice, Clearfield® and Clearfield® Plus sunflower, and Clearfield® and Clearfield® Plus wheat. Imazamox is also used POST at 140-560 g ai/ha for control of float aquatic weeds. Imazamox provided broad spectrum control of broadleaf and grass weeds including redroot pigweed, common cocklebur, common lambsquarters, mustards, nightshade, sunflower, velvetleaf, foxtails, volunteer corn, johnsongrass, shatter cane, and fall panicum. An adjuvant and fertilizer are required for maximum weed efficacy.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: Non-corrosive
Storage stability: Avoid temperatures >40 C. Technical active is not sensitive to oxidizing or reducing agents.
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth of susceptible plants is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by slow, general foliar chlorosis and necrosis.
Absorption/translocation: Generally absorbed rapidly into foliage. Root absorption is slower. Imazamox translocates both in the xylem and phloem. Low translocation in some weed species results from metabolism to non-mobile products.
Metabolism in plants: Soybean tolerance is due to rapid metabolism. Susceptible weed species metabolize imazamox slowly or not at all.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes.

BEHAVIOR IN SOIL

Sorption: Generally weakly bound to soil, but adsorption increases with as clay and OM content increase. Adsorption increases with time and as the soil becomes drier.
Transformation: Primarily degraded by microbes. Imazamox does not degrade appreciably under anaerobic conditions.
Persistence: Average half-life ranges from 20 to 30 d. Imazamox degrades to non-herbicidal products.
Mobility: Field studies indicate that imazamox remains

in the top 30 cm of soil. Field studies do not indicate any potential for imazamox to move with surface water.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade imazamox acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal rabbit LD_{50}, >4000 mg/kg; 4-h inhalation LC_{50} rat, 6.3 mg/L (maximum attainable conc.); Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

1 lb/gal formulation: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >4000 mg/kg; 4-h inhalation LC_{50} rat, 5.0 mg/L (maximum attainable conc.); Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

Subchronic toxicity:

90-d dietary, rat: NOEL 1661 mg/kg/d (HDT)

Chronic toxicity:

18-mo dietary, mouse: NOEL 1201 mg/kg/d (HDT); not oncogenic

Teratogenicity:

Rat: NOEL 500 mg/kg/d (maternal), 1000 mg/kg/d (developmental) (HDT)

Rabbit: NOEL maternal 300 mg/kg/d; fetal 900 mg/kg/d

Reproduction:

Rat: NOEL 1639 mg/kg/d (HDT)

Mutagenicity:

Gene mutation: CHO/HGPRT, negative

Structural chromosome aberration: CHO, negative; Rat bone marrow, negative

DNA damage/repair: Primary rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >5572 mg/kg; Mallard duck 8-d dietary oral LC_{50}, >5572 mg/kg; Honey bee topical LD_{50}, >25 μg/bee; Daphnia 48-h LC_{50}, >122 mg/L; Bluegill sunfish 96-h LC_{50}, >119 mg/L; Rainbow trout 96-h LC_{50}, >122 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 5-hydroxymethyl-2,3 pyridinedicarboxylic acid undergoes dehydration (forms the anhydride), a condensation reaction, and hydrolysis followed by cyclization to form the imidazolinone ring and precipitation as imazamox.

Purification of technical: Technical active ingredient is >95% pure. No further purification is necessary.

Analytical methods: Imazamox is extracted from soybean seed with acidic aqueous methanol and cleaned up via solvent partitioning and solid phase extraction techniques. Imazamox is detected using HPLC equipped with a UV detector. Validated sensitivity of the method is 50 mg/kg. Residues of imazamox and its metabolites are extracted from soil using 0.5 N NaOH. Following precipitation and filtration, the extract is fractionated by differential elution. Residues are detected using HPLC with a UV detector. Validated sensitivity is 0.5 mg/kg for each compound.

Historical: Discovered and developed by American Cyanamid Co. and first registered as RAPTOR in 1997.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF

Reference(s):

1. Shaner, D.L. and S. L. O'Conner. 1991. The Imidazolinone Herbicides. CRC Press, Boca Raton, FL.

imazapic

2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-5-methyl-3-pyridinecarboxylic acid

CAS # Acid: 104098-48-8
or 81334-60-3
NH_4 salt: 104098-49-9

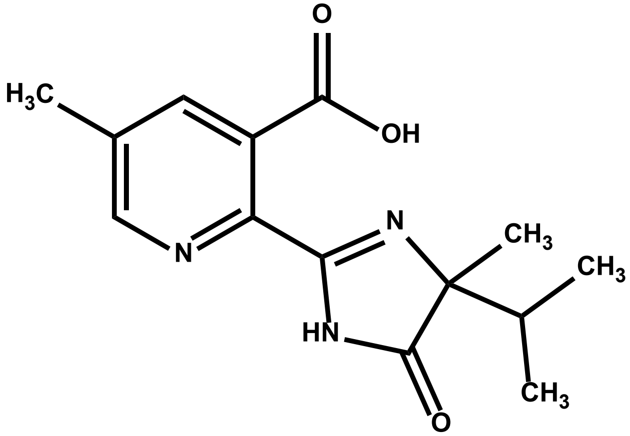
$2^{(B)}$

NOMENCLATURE

Common name: imazapic (WSSA, ISO)
Other name(s): CL 263,222; 2-[(*RS*)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]-5-methylnicotinic acid (IUPAC)
Trade name(s): CADRE®; IMPOSE®; JOURNEY®; PLATEAU®
Chemical family: imidazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
imazapic acid



Molecular formula: *Acid* $C_{14}H_{17}N_3O_3$; *NH_4 salt* $C_{14}H_{20}N_4O_3$
Molecular weight: *Acid* 275.31 g/mole; *NH_4 salt* 292.34 g/mole
Description: Off-white to tan powder, odorless
Density: 0.38 g/mL
Melting point: 204-206 C
Boiling point: NA
Vapor pressure: $<1.3 \times 10^{-5}$ Pa (60 C)
Stability: Stable for >12 mo (37 C)
Solubility:
water 2200 mg/L (25 C)
pK_a: 2.0, 3.9, and 11.1 (weak acid)
K_{ow}: 0.16 (pH 5); 0.01 (pH 7); 0.002 (pH 9)

HERBICIDAL USE

Imazapic can be applied POST at 70 g ae/ha in peanuts. It is also used for selective weeding, grass, forb and brush establishment and turf growth suppression on pastures, rangeland, specified noncrop areas, and conifer plantation site preparation. Imazapic controls many annual broadleaf weeds such as sicklepod, Florida beggarweed, morningglory spp., cocklebur, pigweed spp., common ragweed, prickly sida, lambsquarters, and bristly starbur, and many annual and perennial grasses including *Panicum* spp., johnsongrass, goosegrass, broadleaf signalgrass, foxtail spp., and crabgrass spp., and purple and yellow nutsedge.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: The product CADRE is corrosive to brass, iron, and mild steel.
Storage stability: Shelf life is >12 mo
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth of susceptible plants is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by slow, general foliar chlorosis and necrosis.
Absorption/translocation: Moves in both the xylem and phloem, but primarily the phloem.
Metabolism in plants: Peanut tolerance is due to rapid metabolism, initiated by hydroxylation of the 5-methyl substituent on the pyridine ring followed by glucosylation. Susceptible weed species metabolize imazapic slowly or not at all.
Non-herbicidal biological properties: Imazapic suppresses growth and seedhead production when applied at sublethal rates to certain turf species (bermudagrass and bahiagrass).
Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed in high pH soil, but adsorption increases with lower pH and increasing clay and OM content. Sorption is reversible.
Transformation: Primarily degraded by microbes; Imazapic does not degrade appreciably under anaerobic conditions.
Persistence: Average half-life is 120 d. Planting of certain rotational crops may need to be delayed.
Mobility: Field studies indicate that Imazapic remains in the top 30-45 cm of soil. Field studies do not indicate any potential for imazapic to move with surface water.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade imazapic acid unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal rabbit LD_{50}, >2000 mg/kg; 4-h inhalation LC_{50} rat, >4.83 mg/L (max. attainable

conc.); Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate, reversible

CADRE: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >2.38 mg/L (max. attainable conc.); Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

Subchronic toxicity:

90-d dietary, rat: NOEL 1625 mg/kg/d

21-d dermal, rabbit: NOEL 1000 mg/kg/d

Chronic toxicity:

12-mo dietary, dog: NOEL 160 mg/kg/d; not oncogenic

Teratogenicity:

Rat: NOEL 1000 mg/kg/d

Rabbit: NOEL maternal 500 mg/kg/d, fetal 700 mg/kg/d

Reproduction:

Rat: NOEL 1500 mg/kg/d

Mutagenicity:

Gene mutation: CHO/HGPRT, negative

Structural chromosome aberration: CHO, negative; Rat bone marrow, negative

DNA damage\repair: Primary rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Honey bee topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >100 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L; Channel catfish 96-h LC_{50}, >100 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 5-methyl-2,3 pyridinedicarboxylic acid undergoes dehydration (forms the anhydride), a condensation reaction, and hydrolysis followed by cyclization to form the imidazolinone ring and precipitation as imazapic.

Purification of technical: Technical active ingredient is >95% pure. No further purification is necessary.

Analytical methods: Imazapic residues are extracted from soil using 0.5 N NaOH and clean-up is accomplished with solvent partitioning and solid phase extraction techniques. Imazapic is detected using HPLC equipped with a UV detector. Validated sensitivity of the method is 5 µg/kg. Residues of Imazapic and its metabolites are extracted from plant material using acidic methanol-water and are cleaned-up via solvent partitioning and solid phase extraction techniques. Residues are detected using HPLC with a UV detector. Validated sensitivity is 0.1 µg/kg for each compound.

Historical: Discovered by American Cyanamid Co. in March, 1981. CADRE and PLATEAU were registered in 1996.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF; Adama; Nufarm

Reference(s):

1. Shaner, D. L. and S. L. O'Conner. 1991. The Imidazolinone Herbicides. CRC Press, Boca Raton, FL.

imazapyr

2-[4,5-dihydro-4-methly-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-3-pyridinecarboxylic acid

CAS # Acid: 81334-34-1
Isopropylamine salt: 81510-

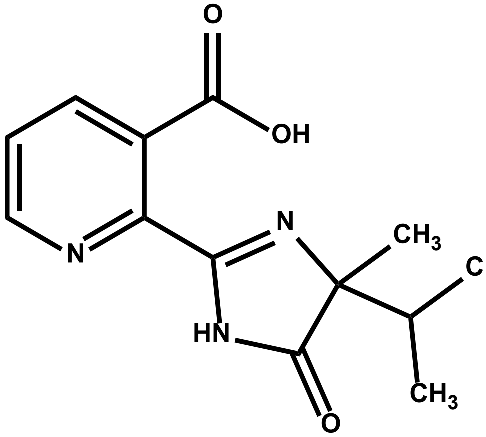
2$^{(B)}$

NOMENCLATURE

Common name: imazapyr (ANSI, BSI, ISO, WSSA)
Other name(s): AC 243,997 (acid); AC 252,925 (isopropylamine (IPA) salt); CL 243,997 (acid); CL 252,925 (IPA salt); 2-[(*RS*)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)nicotinic acid (IUPAC)
Trade name(s): ARES™; ARSENAL®; ARSENAL® AC; ARSENAL® POWERLINE; ARSENAL® RAILROAD; CHOPPER®; CHOPPER® GEN2; HABITAT®; LIGHTNING®; ONESTEP®; SAHARA®; STALKER®
Chemical family: imidazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:



Molecular formula: *Acid* $C_{13}H_{15}N_3O_3$; *IPA salt* $C_{16}H_{24}N_4O_3$
Molecular weight: *Acid* 261.28 g/mole; *IPA salt* 320.39 g/mole
Description: Off-white to tan powder, slight odor
Density: 0.34 g/mL
Melting point: 169-173 C
Boiling point: NA
Vapor pressure: <1.3 x 10^{-5} Pa (45 C)
Stability: Stable for >12 mo (37 C)
Solubility:
water 11,272 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C):
acetone 3.39
dimethyl formamide 30.9
methylene chloride 8.72
ethanol 4.22
methanol 10.5
DMSO 47.1
toluene 0.18
pK$_a$: 1.9, 3.6, and 11.0 (weak acid)
K$_{ow}$: 1.3

HERBICIDAL USE

Imazapyr can be applied to the soil or POST at 0.56-1.7 kg ae/ha, or POST spray-to-wet using 240 - 480 g ae/L on non cropland areas such as fence rows, farm buildings sites, pipeline and highway rights-of-way, utility and pumping installations, roadsides, forestry sites, storage areas, and non-irrigation ditch banks and in imidazolinone-tolerant (Clearfield®) corn in a premix with imazathapyr and certain other Clearfield® and Clearfield® Plus crops. Imazapyr can be applied to establish and maintain wildlife openings, to prepare sites for conifer planting, and to release conifers from competing vegetation. Imazapyr also has been developed for sugarcane and plantation crops such as rubber and oil palm. Imazapyr can also be used to control emergent and floating aquatic vegetation in and around standing and flowing water; wetland, riparian and terrestrial vegetation growing in or around surface water. It controls many annual and perennial weeds including grasses, broadleaves, vines, brambles, brush, and trees. POST application is more effective in most situations. A non-ionic surfactant improves POST efficacy.

USE PRECAUTIONS

Fire hazard: Imazapyr technical (acid) and formulated products are non-flammable.
Corrosiveness: The product ARSENAL is corrosive to iron, mild steel, and brass, but not to #304 stainless steel.
Storage stability: Do not store below 0 C; formulated products are stable for >1 yr.
Cleaning glassware/spray equipment: Wash with water and detergent.
Emergency exposure: Wash skin with soap and water. Flush eyes with water; get medical attention if irritation persists.
Incompatibilities: Reacts with acids or bases and strong oxidants.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth is inhibited within a few h after application, but injury symptoms usually do not appear for 1-2 wk or more. Meristematic areas gradually become chlorotic, followed by a slow foliar chlorosis and necrosis.
Absorption/translocation: Foliar absorption usually is rapid (within 24 h), but may vary with plant species. Imazapyr also is absorbed by roots. It moves readily in both xylem and phloem when root or shoot absorbed.
Metabolism in plants: Tolerance is due to rapid metabolism, initiated by hydroxylation of the imidazolinone ring to form 2-carbamoylnicotinic acid. In this hydrolysis-mediated metabolism, an imidazopyrrolopyridine derivative also is formed. Susceptible weed species metabolize imazapyr slowly or not at all.
Non-Herbicidal biological properties: Sub-lethal rates may be used as a plant growth regulator in certain turf species such as bermudagrass.

Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes (2).

BEHAVIOR IN SOIL

Sorption: Generally weakly bound to soil, but adsorption increases as OM and clay increase. Decreasing pH below 6.5 increases adsorption, although pH increase above 6.5 have little effect. Adsorption increases with time and as soil dries. Sorption is reversible.

Transformation:

Photodegradation: Half-life in water is 1-2 d when exposed to a xenon arc lamp, producing quinolinic acid, quinolinimide, and furo[3,4-*b*]pyridine-5(7*H*)-one and 7-hydroxy-furo[3,4-*b*]pyridine-5(7*H*)-one. Photolysis on the soil surface is limited and is a minor contributor to degradation in soil.

Other degradation: Microbial degradation is the prinicipal means of imazapyr dissipation in soil. Anaerobic microbial degradation occurs at much slower rates.

Persistence: Field half-life ranges from 25 to 142 d depending on soil characteristics and environmental conditions. Weed control efficacy persists from 3 mo to 2 yr depending on application rate. Half-life in shallow ponds ranged from 2 to 3 d.

Mobility: Imazapyr generally remains within the top 50 cm of soil in field dissipation studies. In forest dissipation studies, imazapyr did not run off into streams, and no evidence of lateral movement was observed.

Volatilization: Insignificant losses

Formulation effects: Environmental fate appears similar between liquid and granular formulations.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade imazapyr acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >1.3 mg/L (maximum attainable dose); Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, irreversible

ARSENAL: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >2.38 mg/L (maximum attainable dose); Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

Subchronic toxicity:

90-d dietary, rat: NOEL 500 mg/kg/d

90-d dietary, dog: NOEL 250 mg/kg/d

21-d dermal, rabbit: 400 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 1500 mg/kg/d; not oncogenic

24-mo dietary, rat: NOEL 500 mg/kg/d; not oncogenic

12-mo dietary, dog: 400 mg/kg/d

Teratogenicity:

Rat: NOEL maternal 300 mg/kg/d, fetal 1000 mg/kg/d; not teratogenic

Rabbit: NOEL 400 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 500 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative; *E. coli*, negative; CHO/HGPRT, negative

Structural chromosome aberration: CHO, negative; Rat dominant lethal, negative

DNA damage/repair: Primary rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Honey bee topical LD_{50}, >100 μg/bee; Daphnia 48-h LC_{50}, >100 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Channel catfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 2, 3 pyridinedicarboxylic acid undergoes dehydration (to form the anhydride), a condensation reaction, hydrolysis, is cyclized (to form the imidazolinone ring), and is precipitated as the manufacturing use product.

Purification of technical: Synthesis during manufacture results in technical active ingredient with a purity >95%. No additional purification is needed.

Analytical methods: Residues in soil are extracted with 0.5 N NaOH, followed by clean-up with solid phase extraction techniques. Residues are quantified by HPLC with a UV detector (240 nm). Validated sensitivity of the method is 5 μg/kg.

Historical: Discovered by American Cyanamid Company in the late 1970s. Testing begun in 1981 indicated potential as an herbicide for total vegetation control. Subsequent research demonstrated tolerance in several pine species, prompting development as a forestry herbicide. Commercial sales of imazapyr began in 1984. First reported in 1983 (1).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF; Nufarm; PBI Gordon

Reference(s):

1. Orwick, P.L. et al. 1983. Proc. South. Weed Sci. Soc. 36:291.
2. Shaner, D.L. and S. L. O'Conner. 1991. The Imidazolinone Herbicides. CRC Press, Boca Raton, FL.
3. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

imazaquin

CAS #: 120923-37-7 **$2^{(B)}$**

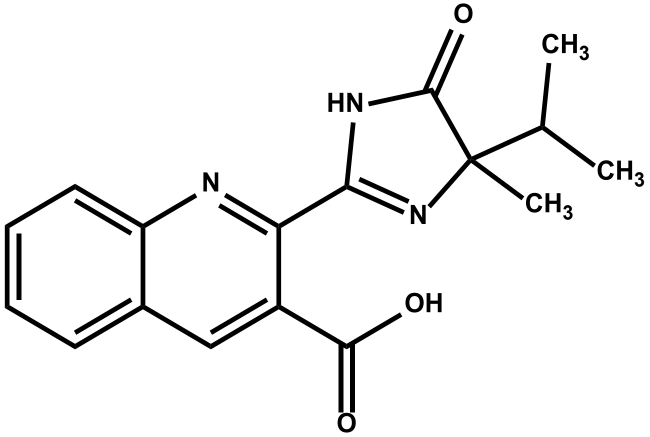
2-[4,5-dihydro-4-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-3-quinolinecarboxylic acid

NOMENCLATURE

Common name: imazaquin (ANSI, BSI, ISO, WSSA)
Other names: AC 252,214; CL 252,214; imazaquin; 2-[(RS)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]quinoline-3-carboxylic acid (IUPAC)
Trade name(s): IMAGE®; SCEPTER®
Chemical family: imidazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: imazaquin acid



Molecular formula: Acid $C_{17}H_{17}N_3O_3$; NH_4 salt $C_{17}H_{20}N_4O_3$
Molecular weight: Acid 311.34 g/mole; NH_4 salt 328.37 g/mole
Description: Tan solid, slightly pungent odor
Density: 0.39 g/mL untapped; 0.43 g/mL tapped
Melting point: 219-224 C
Boiling point: NA
Vapor pressure: $<1.3 \times 10^{-5}$ Pa
Stability: Stable for >24 mo (25 C); decomposes at 219-224 C
Solubility:

Acid
water 60 mg/L (25 C)
organic solvents g/100 mL (25 C)
acetone 0.3
dimethylformamide 6.8
DMSO 15.9
ethanol 0.06
heptane 0.02
methanol 0.5
methylene chloride 1.4
toluene 0.04

Ammonium salt
water 160,000 mg/L (20 C) and pH 7 (4)

pK_a: 3.8 (weak acid)
K_{ow}: 2.2 (22 C)

HERBICIDAL USE

Imazaquin can be applied preplant surface, PPI, or PRE at 105 or 140 g ae/ha or POST at 70 or 140 g/ha in soybeans. Soil-applied imazaquin controls certain annual grasses and many annual broadleaf weeds including foxtails, seedling johnsongrass, cocklebur, jimsonweed, lambsquarters, POST-applied imazaquin controls volunteer corn, cocklebur, pigweeds, wild poinsettia, morningglory spp and common sunflower. Imazaquin can be impregnated on dry bulk fertilizer. A nonionic surfactant or oil adjuvant improves efficacy of POST applications. Some rotational crops such as barley, cotton, corn, oats, and sugarbeets are susceptible to imazaquin residues in the soil. Can also be used for broadleaf weed and nutsedge control in established and selected turfgrasses and around selected landscape ornamentals.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: The product SCEPTER and IMAGE aqueous formulations are corrosive to mild steel, brass, copper, zinc, and iron, but non-corrosive to stainless steel.
Storage stability: Shelf life is 2 yr for SCEPTER and IMAGE aqueous formulations, and >2 yr for SCEPTER DG and IMAGE DG.
Cleaning glassware/spray equipment: Wash with water.
Incompatibilities: Tank mixing with postemergence grass herbicides antagonizes grass control; incompatible with strong oxidants.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by a slow general foliar chlorosis and necrosis.
Absorption/translocation: Readily absorbed by foliage and roots, with most rapid uptake occurring via roots. Differential absorption may occur among species, and decreased foliar absorption may account for the greater susceptibility in cocklebur compared to velvetleaf. Imazaquin is translocated in both xylem and phloem, but primarily the phloem. Translocation is decreased in some species due to metabolism to non-mobile products and may be responsible for decreased susceptibility.
Metabolism in plants: Soybean rapidly metabolize imazaquin. The metabolic pathway includes ring closure of the carboxyl group with the imidazolinyl nitrogen and hydrolysis of the acetamide and carbamoyl moieties of the metabolite. Susceptible species such as cocklebur metabolize imazaquin slowly or not at all.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes (2).

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed in high pH soil, but adsorption increases in soil with lower pH. Most sorption is reversible.

K_{oc}: 20 mL/g (estimated) at pH 7 (4), but varies with pH

Transformation:

Photodegradation: Photolysis is the major means of degradation in aquatic systems, with half-lives of <1 d (8-21 h depending on pH) at 18-19 C and four products identified: 3-quinoline-carboxylic acid; 2,3-quinoline-dicarboxylic acid; 2-carboxamido-3-quinolinecarboxylic acid; and 2,3-dihydro-3-imino-1H-pyrrolo[3,4-b]quinoline-1-one. Photolysis on dry soil surfaces is much slower than in aqueous solution, with half-lives of several mo and no major products formed. Photolysis on dry soil generally contributes little to imazaquin degradation, but this may vary with environmental conditions.

Other degradation: Primarily degraded in soil by microbial action. Soil degradation studies with ^{14}C label on either the carboxyl carbon or the quinoline ring yielded no major metabolites except CO_2. Degradation rate is higher with higher soil temperature and moisture, although temperatures beyond a certain point will not further increase and may decrease degradation rate. Non-microbial degradation (except photolysis) appears to be insignificant. Imazaquin has a low potential for forming bound residues.

Persistence: Average field half-life is 60 d (4). However, half-lives in many southern states may be ~1 mo with longer half-lives generally observed in northern states. Planting of certain rotational crops may need to be delayed.

Lab experiments: Most half-lives are 2-4 mo, but range from 1.3 to 12 mo depending on incubation conditions.

Mobility: In field studies, imazaquin remains in the top 30 cm of soil, and has shown no potential for movement with surface water.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade imazaquin acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg, female mouse, 2363 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.7 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, none

SCEPTER: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >1.49 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

SCEPTER 70DG: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL 831 mg/kg/d

21-d dermal, rabbit: 1000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 150 mg/kg/d

24-mo dietary, rat: NOEL 500 mg/kg/d

12-mo dietary, dog: 25 mg/kg/d

Teratogenicity:

Rat: NOEL maternal 500 mg/kg/d

Rabbit: NOEL maternal 250 mg/kg/d, fetal 500 mg/kg/d

Reproduction:

Rat: NOEL 1000 mg/kg/d in a 3-generation study

Mutagenicity:

Gene mutation: Ames test, negative; E. coli, negative; CHO negative

Structural chromosome aberration: CHO, negative; Rat dominant lethal, negative

DNA damage/repair: Primary rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000; Honey bee topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >100 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L; Channel catfish 96-h LC_{50}, >100 mg/L

Use classification: General use for most products

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 2,3-quinoline-dicarboxylic acid undergoes dehydration (to form the anhydride), a condensation reaction, hydrolysis, is cyclized (to form the imidazolinone ring), and is precipitated as the manufacturing use product.

Purification of technical: Synthesis during manufacture results in technical active ingredient with a purity >95%. No additional purification is needed.

Analytical methods: Residues in soil are extracted with 0.5 N NaOH in 30% methanol, followed by clean-up with solid phase extraction cartridges, and by solvent partitioning. Residues are quantified by liquid chromatography with a UV detector (240 nm). Validated sensitivity of the method is 5 µg/kg. Imazaquin residues are extracted from soybean tissue using acidic methanol-water and extracts are cleaned-up via solvent partitioning and solid phase extraction techniques. Residues are quantified with on-column methylation and GC using a nitrogen-sensitive detector. Validated sensitivity of the method is 0.05 µg/g.

Historical: Discovered by American Cyanamid Company in 1980 and was the first imidazolinone herbicide to be widely used. Field testing began in 1981 followed by a Section 18 Emergency Exemption in 1985 for control of sicklepod in five southern states. Imazaquin was first reported in 1983 (2), and was first registered in 1984 on soybeans in Argentina, followed by U.S. registration in 1986.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF

Reference(s):

1. Orwick, P.L. et al. 1983. Abst. Weed Sci. Soc. Am. 18.
2. Shaner, D.L. and S. L. O'Conner. 1991. The Imidazolinone Herbicides. CRC Press, Boca Raton, FL.
3. Shaner, D. L. et al. 1984. Plant Physiol. 76:545.
4. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

imazethapyr

2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1*H*-imidazol-2-yl]-5-ethyl-3-pyridinecarboxylic acid

CAS # Acid: 81335-77-5
NH_4 salt: 101917-66-2

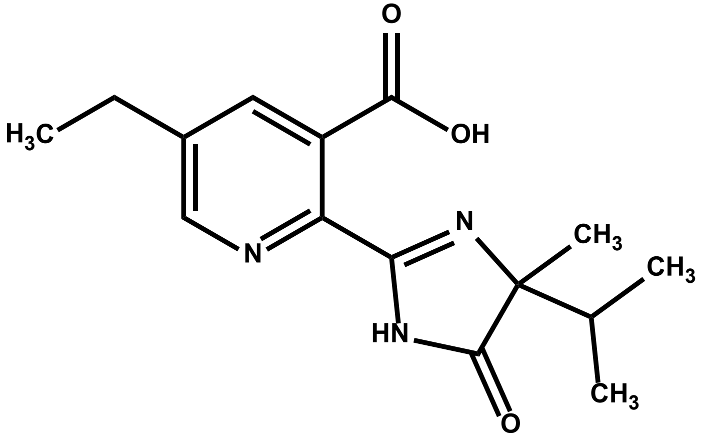
2$^{(B)}$

NOMENCLATURE

Common name: imazethapyr (ANSI, BSI, ISO, WSSA)
Other name(s): AC 263,499; CL 263,499; 5-ethyl-2-[(RS)-4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl]nicotinic acid (IUPAC)
Trade name(s): ABSOLUTE®; ASSIGNMENT®; CLEAN SWEEP®; CLEARPATH®; CONQUEST® LQ; EXTREME®; LIGHTNING®; NEWPATH®; ODYSSEY®; OPTILL®; OPTILL® PRO; PURSUIT®; PURSUIT® PLUS
Chemical family: imidazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *imazethapyr*



Molecular formula: *Acid* $C_{15}H_{19}N_3O_3$; *NH_4 salt* $C_{15}H_{22}N_4O_3$
Molecular weight: *Acid* 289.33 g/mole; *NH_4 salt* 306.36 g/mole
Description: Off-white to tan solid, slightly pungent odor (technical)
Density: 1.10-1.12 g/mL (21 C)
Melting point: 169-173 C
Boiling point: Decomposes before boiling (180 C)
Vapor pressure: 1.3 x 10^{-5} Pa
Stability: Decomposes at 180 C
Solubility:
water 1400 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C)

acetone 4.82	methylene chloride 1.4
DMSO 42.25	2-propanol 1.73
heptane 0.09	toluene 0.5
methanol 10.5	

pK_a: 2.1 and 3.9 (weak acid)
K_{ow}: 11 (pH 5); 31 (pH 7); 16 (pH 9)

HERBICIDAL USE

Imazethapyr can be applied as follows: POST at 53-70 g ae/ha in soybeans; early preplant, PPI, PRE, and POST at 70 g ae/ha in soybeans and imidazolinone-resistant crops such as Clearfield® corn and Clearfield® canola; PPI, PRE, or POST at 35-53 g ae/ha in edible legumes; at 70 g ae/ha on Conservation Reserve Program (CRP) land; and POST at 70-105 g ae/ha in alfalfa; PPI, PRE, at-cracking, and POST at 70 g ae/ha in peanuts. Imazethapyr can also be applied to Clearfield® rice at 70 g/ha PRE followed by 70 g/ha POST for control of red rice. Split applications in peanuts allow 35 g ae/ha soil-applied followed by 35 g ae/ha at-cracking or POST. Imazethapyr controls many annual broadleaf weeds including bristly starbur, buffalobur, cocklebur, jimsonweed, kochia, lambs-quarters, smallflower morningglory, nightshade spp., pigweed spp., ragweed spp., spurge spp., spurred anoda, sunflower, and velvetleaf along with several annual grasses such as barnyardgrass, large crabgrass, broadleaf signalgrass, fall panicum, seedling johnsongrass, and red rice, rice flatsedge, shattercane, as well as nutsedge spp. A non-ionic surfactant, oil adjuvant, or fertilizer adjuvant is required for maximum POST efficacy.

USE PRECAUTIONS

Fire hazard: The product PURSUIT is non-flammable; flash point is >93 C (>199 F).
Corrosiveness: The product PURSUIT is corrosive to zinc, mild steel, brass, copper, and aluminum, but non-corrosive to #304 stainless steel.
Storage stability: Do not store PURSUIT below 0 C or PURSUIT PLUS below 4 C. All products are stable for >1 yr after manufacture.
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent.
Incompatibilities: Incompatible with strong oxidants

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth is inhibited within a few h after application, but injury symptoms usually appear after 1-2 wk or more. Meristematic areas become chlorotic, followed by a slow general foliar chlorosis and necrosis.
Absorption/translocation: Generally absorbed rapidly into foliage, although absorption varies from 20 to 90% in 24 h. Root absorption is slower. Imazethapyr translocates in both xylem and phloem, but primarily the phloem. Low translocation in some weed species results from metabolism to non-mobile products.
Metabolism in plants: Soybean tolerance is due to rapid metabolism, initiated by oxidative hydroxylation at the α-carbon of the 5-ethyl substituent on the pyridine ring, followed by glucose conjugation. Sensitive weed species metabolize imazethapyr slowly or not at all.
Non-herbicidal biological properties: Imazethapyr plus imazapyr is used at sub-lethal rates as a turfgrass growth suppressant.

Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes (2).

BEHAVIOR IN SOIL

Sorption: Binding of imazethapyr to soil generally is weak, although adsorption increases as OM and clay increase; decreasing pH below 6.5 increases binding, whereas adsorption changes little from pH 6.5-8; Adsorption increases with time and as soil becomes drier. Sorption is reversible.

Transformation

Photodegradation: Half-life in distilled water is 46 h when exposed to light from a xenon arc lamp filtered through borosilicate glass. The principal degradation products identified were 5-ethyl-2,3-pyridinedicarboxylic acid and 5-ethyl-3-pyridinecarboxylic acid. Photolysis on soil surfaces is limited.

Other degradation: Primarily degraded by microbes. Essentially no degradation occurs under anaerobic conditions.

Persistence: Typical field half-life is 60-90 d. Planting of certain rotational crops may need to be delayed.

Mobility: Imazethapyr remains in the top 30 cm of soil. Field studies suggest no potential for movement with surface water.

Volatilization: Insignificant losses

Formulation effects: Environmental fate properties are unaffected by formulation type.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade imazethapyr acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >3.27 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

PURSUIT: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >2.67 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

Metabolism in plants: Soybean tolerance is due to rapid metabolism, initiated by oxidative hydroxylation at the ⟨-carbon of the 5-ethyl substituent on the pyridine ring, followed by glucose conjugation. Sensitive weed species metabolize imazethapyr slowly or not at all.

Non-herbicidal biological properties: Imazethapyr plus imazapyr is used at sub-lethal rates as a turfgrass growth suppressant.

Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes (2).

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 5-ethyl-2,3 pyridinedicarboxylic acid undergoes dehydration (to form the anhydride), a condensation reaction, and hydrolysis followed by cyclization to form the imidazolinone ring, and precipitation as the manufacturing use product.

Purification of technical: Synthesis during manufacture results in technical active ingredient with a purity >95%. No additional purification is needed.

Analytical methods: Imazethapyr residues are extracted from soil using 0.5 N NaOH. Clean-up is accomplished with solvent partitioning and solid phase extraction techniques. Imazethapyr is measured using HPLC equipped with a UV detector. Validated sensitivity of the method is 5 μg/kg. Residues of imazethapyr and its metabolites are extracted from plant material using acidic methanol-water and are cleaned-up via solvent partitioning and solid phase extraction techniques. Residues are measured with on-column methylation and GC equipped with a nitrogen-sensitive detector. Validated sensitivity of the method is 50 μg/kg for each compound.Cyanamid Company in April, 1981. It was first tested on soybeans under an Experiment Use Permit (EUP) in 1987-88. The EPA granted a FIFRA Section 18 (Emergency Exemptions) for use on soybeans in 1987-88 and for edible beans in 1987-88. EPA issued full registration for soybeans in 1989, edible beans and peas in 1990, peanuts in 1991, and imidazolinone-tolerant corn in 1992. First reported in 1984 (1).

Historical: Imazethapyr was discovered by American Cyanamid in 1981.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; Albaugh, Inc./Agri Star; BASF; Cheminova; FMC; Loveland; PBI Gordon

Reference(s):

1. Malefyt, T. et al. 1984. Abstr. Weed Sci. Soc. Am. 18.
2. Shaner, D. L. and S. L. O'Connor. 1991. The Imidazolinone Herbicides. CRC Press, Boca Raton, FL.

imazosulfuron

CAS #: 122548-33-8 **2$^{(B)}$**

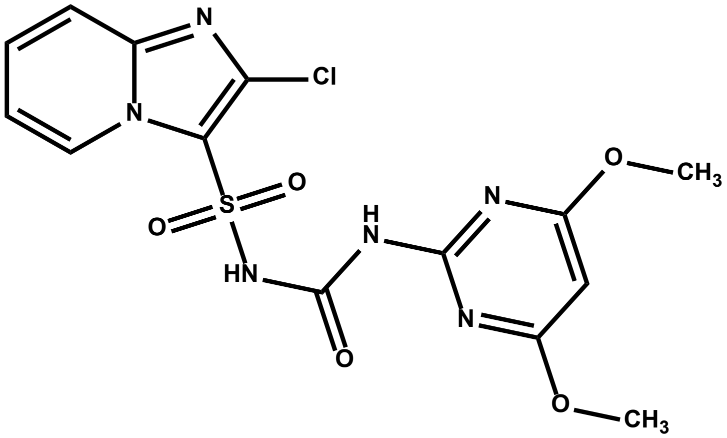
2-chloro-*N*-[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]
imidazo[1,2-*a*]pyridine-3-sulfonamide

NOMENCLATURE

Common name: imazosulfuron (ISO 1750 published)
Other name(s): LGC-42153; TH-913; 1-(2-chloroimidazo[1,2-*a*]pyridin-3-ylsulfonyl)-3-(4,6-dimethoxypyrimidin-2-yl)urea (IUPAC)
Trade name(s): SIBATITO; TAKEOFF
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
imazosulfuron



Molecular formula: $C_{14}H_{13}ClN_6O_5S$
Molecular weight: 412.81 g/mole
Description: Crystalline powder
Density: 1.54 g/mL (25 C)
Melting point: 183-184 C (decomposition)
Boiling point: NA
Vapor pressure: 4.0 x 10^{-2} Pa (20 C)
Stability: NA
Solubility:
water 6.75 mg/L (pH 5.1; 25 C); 67 mg/L (pH 6.1; 25 C); 308 mg/L (pH 7.0, 25 C)
organic solvents (g/L at 99.9% purity and 20 C):

dicloromethane 12.9	acetonitrile 2.5
acetone 4.2	xylene 0.4
ethylacetate 2.1	methanol 0.13

pK_a: 4.0 (20 C) (weak acid)
K_{ow}: log K_{ow} = 1.88 (pH 4); 1.59 (pH 7);> 0.29 (22 C)

HERBICIDAL USE

Postemergence herbicide for annual and perennial broadleaf weeds and sedge in paddy rice (75-95 g ai/ha) and turf (500-1000 g ai/ha).

USE PRECAUTIONS

Fire hazard: Formulated product is non-flammable
Corrosiveness: Non-corrosive
Storage stability: Keep container tightly closed in a cool, dry place
Emergency exposure: Emergency exposure: On ingestion, to not induce vomiting. Dilute swallowed product with large amounts of water. On eye contact, flush with water for at least 15 min. On skin contact, flush with water for at least 15 min. On inhalation, move victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth of treated plants is inhibited within a few h after application, but injury symptoms usually appear 1-2 wk later. Meristematic areas gradually become chlorotic and necrotic, followed by a general foliar chlorosis and necrosis.
Absorption/translocation: Absorption/translocation: Rapid foliar and root absorption; primarily transported in the phloem and accumulates in meristematic areas.
Metabolism in plants: *O*-demethylation of imazosulfuron was the primary metabolic reaction in excised pea root, rice leaves, and *Cyperus serotinus*.
Mechanism of resistance in weeds: Altered herbicide binding site in the ALS target enzyme

BEHAVIOR IN SOIL

Soil Sorption:
K_f: 1.46-3.02 mLs/g; retention increases with increasing organic matter and acidic soil pH
Mobility: Residues confined mainly to top layer of soil
Transformation:
Photodegradation: pH 5.5, imazosulfuron half-life was 90 min at 254 nm and 480 min at >290 nm
Other degradation: Hydrolysis is characterized by first-order kinetics, pH- and temperature-dependent, and accelerated by acidic conditions and higher temperatures. Hydrolysis DT_{50} was 36.5 and 578 days at pH 4.5 and 5.9, respectively. At pH 6.6, 7.4, 9.2, and 12.3, no change in imazosulfuron concentration was observed after 150 days. A 3 to 5-fold increase in the rate of hydrolysis was found for each 10 C increase in temperature.
Persistence:
Field persistence: DT_{50} is 70 d in aerobic and anaerobic conditions
Lab experiments: DT_{50} 11-120 d
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade imazosulfuron unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat > 5000 mg/kg; Dermal LD_{50} rat > 2000 mg/

kg; Acute dermal LC_{50} rat (4 h) > 25.4 mg/L; Non-irritating to skin or eyes (rabbits); not a skin sensitizer (guinea pig)

Chronic toxicity:

NOEL (2-yr) 106.1 mg/kg (male); 132.46 mg/kg (female) rats; 1-yr 75 mg/kg for male and female dogs; not oncogenic or teratogenic in rats and mice

Teratogenicity: NA

Wildlife:

Mallard duck and bobwhite quail oral LD_{50}, >2250 mg/kg; honey bee LD_{50} (48 h oral), >48.2 µg/bee; carp (48 h) LC_{50}, >10 mg/L; Daphnia magna LC_{50} (3 h), >40 mg/L

Mutagenicity: NA

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Historical: Discovered by Takeda Agro. Co; not sold in the United States and Canada

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Sumitomo Chemical; Takeda Agro Co.

Reference(s):

1. Tomlin, C.D.S. 1997. The Pesticide Manual, Eleventh Edition. BCPC.
2. Morrica, P., F. Barbato, R. Iacovo, S. Seccia, and F. Ungaro. 2001. Kinetics and mechanism of imazosulfuron hydroloysis. J. Food Agric. Chem. 49: 3816-2820.
3. Morrica, P., F. Barbato, R. Iacovo, S. Seccia, and F. Ungaro. 2000. Adsorption and desorption of imazosulfuron by soil. J. Food Agric. Chem. 48: 6132-6137.
4. Morrica, P., A. Giordana, S. Seccia, F. Ungaro, and M. Ventriglia. 2003 Degradation of imazosulfuron in soil. Pest Manag. Sci. 57: 360-365.
5. Morrica, P., P. Fidente, and S. Seccia. 2004. Identification of photoproducts from imazosulfuron by HPLC. Biomedical Chromatog. 18: 450-456.
6. Kim, J., K. H. Liu, S.H. Kang, S.J. Koo, and J.H. Kim. 2003. Degradation of the sulfonylurea herbicide LGC-42153 in flooded soil. Pest Manag. Sci. 59: 1037-1042.
7. Roberts, T. R. 1998. Metabolic Pathways of Agrochemicals, Pt. 2. Royal Society of Chemistry.

indaziflam

CAS #: 950782-86-2

29$^{(L)}$

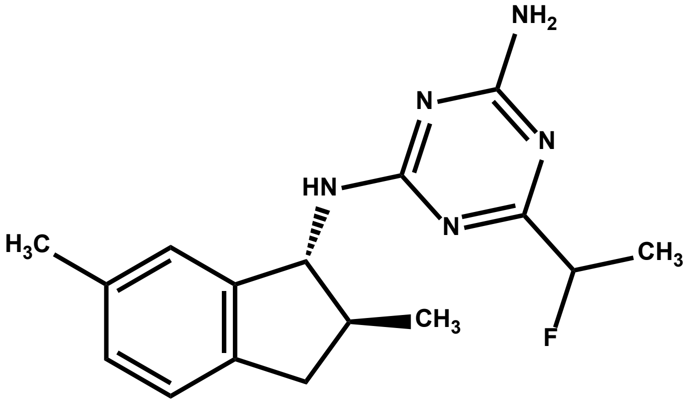
N-[(1*R*,2*S*)-2,3-dihydro-2,6-dimethyl-1*H*-inden-1-yl]-6-(1-fluoroethyl)-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: indaziflam (ANSI, ISO, WSSA)
Other name(s): *N*-[(1*R*,2*S*)-2,3-dihydro-2,6-dimethyl-1*H*-inden-1-yl]-6-[(1*RS*)-1-fluoroethyl]-1,3,5-triazine-2,4-diamine (IUPAC)
Trade name(s): ALION HERBICIDE; SPECTICLE; DURAZONE, ESPLANADE; MARENGO.
Chemical family: fluoroalkyltriazine; alkylazines

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
indaziflam



Molecular formula: $C_{16}H_{20}FN_5$
Molecular weight: 301.36 g/mole
Description: Light brown solid
Density: 1.23 g/cm^3 at 20 C
Melting point: 183 -184 C
Boiling point: NA
Vapor pressure: 6.8 x 10^{-8} PA Pa (25 C); Henry's Law constant, 2.69 x 10^{-6} [Pa x m^3/mol] at 20 C
Stability: Stable
Solubility:
water: 2040 mg/L (pH 7, 25 C); 18,300 mg/L (pH 9, 25 C)
organic solvents g/L (25 C):

acetone	55
heptane	0.032
acetonitrile	7.6
ethanol	13.0
dichloromethane	150
ethyl acetate	47

pK$_{a}$:weak acid.
K$_{ow}$: 2.0 (pH 2); 2.8 (pH 4, pH 7, and pH 9)

HERBICIDAL USE

Indaziflan is registered to control annual grasses and broadleaf weeds in pome fruit, stone fruit, grapes, tree nuts and turf at a rate of 25-100 g/ha.

USE PRECAUTIONS

Fire hazard: Non-flammable.
Corrosiveness: The product is non-corrosive.
Storage stability: Stable
Cleaning glassware/spray equipment: Thoroughly clean all mixing and spray equipment, including tanks, pumps, nozzles, lines, filters, screens and nozzles with a good quality tank cleaner.
Emergency exposure: May irritate eyes, nose, throat, and skin
Incompatibilities: NA.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of cellulose biosynthesis.
Symptomology: Appplied preemergence results in the inability of weed seedlings to grow. Applied postemergences symptoms inclued stunted growth and root swelling or clubbing.(more details on page 16)
Absorption/translocation: NA
Metabolism in plants: NA
Non-herbicidal biological properties: None of significant value
Mechanism of resistance in weeds: No known resistance..

BEHAVIOR IN SOIL

Sorption:
K$_{oc}$: >1000 (1)
Transformation:
Photodegradation: Negligible losses
Other degradation: Indaziflam dissipates in the environment primarily through biotic degradation and leaching. The major transformation products resulting from the environmental degradation of indaziflam are: triazine-indanone; indaziflam-carboxylic acid; indaziflam-hydroxyethyl; indaziflam-olefin; fluoroethyldiaminotriazine; and fluoroethyltriazinanedione.
Persistence: Long resisdual with an average half life >150 d.
Mobility: NA
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade indaziflan unless otherwise indicated.

Acute toxicity:
Oral LD$_{50}$ rat, >2000 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; 4-h inhalation LC$_{50}$ rat, >2.3 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none
Subchronic toxicity:
90-d dietary, rat: NOAEL = 14/410 mg/kg/day; LOAEL = 338/806 mg/kg/day
90-d dietary, dog: NOAEL = 7.5 mg/kg/day; LOAEL = 15 mg/kg/day,

Chronic toxicity:

9-mo dietary, rat: NOAEL: 19 mg/kg/day; LOAEL: 185 mg/kg/day
12-mo dietary, dog: NOAEL: 2.0 mg/kg/day LOAEL: 6/7 mg/kg/day

Teratogenicity:NA

Reproduction:
Rat: NOAEL: 69.3/85.2 mg/kg/day

Mutagenicity:
Gene mutation: Ames test, negative; CHO, negative
Structural chromosome aberration: negative
DNA damage/repair: negative

Wildlife:
LD50/LC50 > 2,000 mg a.i./L for mallard duck; non-toxic to bees and earthworms

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA.
Historical: Indaziflam was first introduced in 2010 for use in turf.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
References:

1. http://www.epa.gov/pesticides/chem_search/reg_actions/registration/fs_PC-080818_26-Jul-10.pdf

iodosulfuron

4-iodo-2-[[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino] carbonyl]amino]sulfonyl] benzoic acid

CAS # Acid: 185119-76-0
Methyl-sodium: 144550-36-7

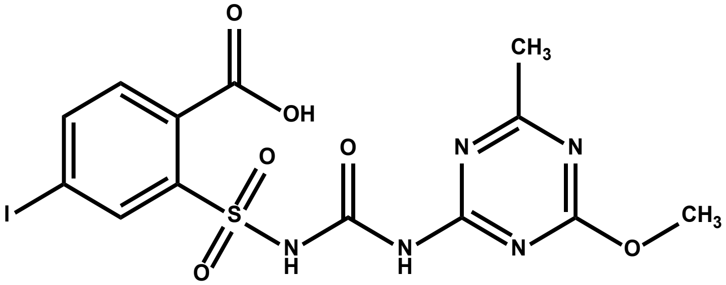
2$^{(B)}$

NOMENCLATURE

Common name: iodosulfuron (ISO-approved)
Other name(s): AEF 115008; 4-iodo-2-[3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)ureidosulfonyl]benzoic acid (IUPAC)
Trade name(s): AUTUMN™; HUSSAR®; CHEKKER®; HUSAR®; SEKATOR®
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *iodosulfuron*



Molecular formula: $C_{13}H_{12}IN_5O_6S$
Molecular weight: 529.24 g/mole
Description: light beige crystalline powder
Density: 0.7 g/mL
Melting point: 152 C
Boiling point: NA
Vapor pressure: 6.7×10^{-9} Pa (25 C)
Stability: Abiotic hydrolysis (pH 5, 20 C) DT_{50} 32; (pH 7, 20 C) >365 d; (pH 9, 20 C) 362 d.
Solubility:
water, 0.16 g/L (pH 5, 20 C); 25 g/L (pH 7, 20 C); 65 g/L (pH 9, 20 C)
pK_a: 3.22 (weak acid)
K_{ow}: log K_{ow} = 1.07 (pH 5); -0.70 (pH 7); -22 (pH 9)

HERBICIDAL USE

Iodosulfuron is used for post-emergence control of broadleaf weeds in cereals, corn, and rice. It is formulated with the safener mefenapyr-diethyl for use on cereals. It has also been combined with amidosulfuron and fenoxaprop-p-ethyl.

USE PRECAUTIONS

Fire hazard: Non-flammable; avoid build up of dust as a dust/air mixture can be explosive
Corrosiveness: Non-corrosive
Storage stability: Stable under normal conditions
Emergency exposure: Rinse eyes immediately with clean water for at least 15 min. and obtain urgent medical aid; if swallowed, wash out mouth with water
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Chlorosis of meristematic tissue followed by necrosis and plant death.
Absorption/translocation: Iodosulfuron is absorbed by roots and foliage. Translocation occurs primarily in the phloem.
Metabolism in plants: NA
Mechanism of resistance in weeds: Altered site of action

BEHAVIOR IN SOIL

Sorption:
K_{oc}:10-90 mLs/g
Transformation:
Photodegradation: DT_{50} 50 d at 52° N latitude
Persistence:
Field experiments: DT_{50} 1-5 d; low soil moisture extends DT_{50} to 7-10 d
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise stated.
Acute toxicity:
Oral LD_{50} rat, 2678 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; non-irritating to skin and eyes
Mutagenicity: Non-mutagenic
Wildlife:
96-h LC_{50} for rainbow trout and bluegill sunfish, >100 mg/L; 48-h EC_{50} for Daphnia magna, >100 mg/L; Acute oral LD_{50} for Japanese quail, bobwhite quail and mallard duck, >2000 mg/kg; 72-h EC_{50} for green algae, 0.07 mg/L
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1. Hacker, E., H. Bieringer, L. Willms, O. Ort, H. Koecher, H. Kehne, and R. C. Fisher. 1999. Iodosulfuron plus mefenpyrdiethyl – a new foliar herbicide for weed control in cereals. Proc. Br. Corp Prot. Conf. – Weeds Vol. 1:15-22.

ioxynil

4-hydroxy-3,5-diiodobenzonitrile

CAS # Acid: 1689-83-4
Na salt: 2961-62-8
Octanoate ester: 3861-47-0

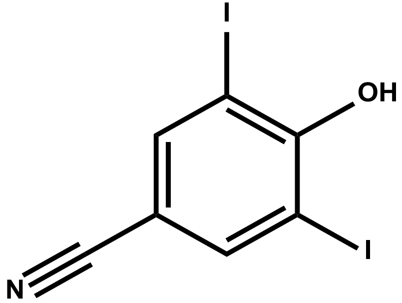
$6^{(C_3)}$

NOMENCLATURE

Common name: ioxynil (BSI, ISO, WSSA)
Other name(s): ACP 63; ACP 63-303; MB 8873; 4-cyano-2,6-diiodophenyl octanoate; 4-hydroxy-3,5-diiodobenzonitrile (IUPAC); 4-hydroxy-3,5-diiodophenyl cyanide (IUPAC)
Trade name(s): ACTRIL DS; BELGRAM; DICTATOR B; DOUBLET; FOXPRO DT; FOXTRIL SUPER; OXYTRIL; OXYTRIL M; IOTRIL®; SPRINGCLENE; TOTRIL; TWINTAK
Chemical family: benzonitrile; hydroxybenzonitrile; nitrile

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
ioxynil acid



Molecular formula: *Acid* $C_7H_3I_2NO$; *Na salt* $C_7H_2I_2NNaO$; *Octanoate ester* $C_{15}H_{17}I_2NO_2$
Molecular weight: *Acid* 370.92 g/mole; *Na salt* 392.90 g/mole; *Octanoate ester* 497.11 g/mole
Description: *Acid* Light buff to creamy powder, odorless when pure; *Octanoate ester* Cream-colored, waxy solid
Density: NA
Melting point: *Acid* 212-213 C; *Octanoate ester* 59-60 C
Boiling point: NA
Vapor pressure: <1 x 10^{-3} Pa (20 C)
Stability: Decomposed by UV light; Slight decomposition above boiling point
Solubility:

Acid
water 130 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone >10
benzene 1.1
carbon tetrachloride 0.14
methanol 3.3

Sodium salt
water 14 mg/L (20-25 C)
organic solvents g/100 mL (20-25 C):
acetone 12
methoxyethanol 64
tetrahydrofurfuryl alcohol 65

Octanoate ester
water insoluble (20-25 C)
organic solvents g/100 mL (20-25 C):
acetone 10
benzene 65
ethanol 8
methanol 9
carbon tetrachloride 60
chloroform 65
cyclohexanone 50
methylene chloride 70
naphtha 70
n-propanol 15

pK_a: 3.96 (weak acid)
K_{ow}: NA

HERBICIDAL USE

Ioxynil can be applied POST in fall-seeded small grains, onions, poppies, rice, sugarcane, flax, and pastures. It is applied alone in onions or tank mixed with other broadleaf herbicides in the other crops. Typical rates in mixture with bromoxynil are 0.2 + 0.2 kg/ha. Ioxynil controls weeds in the Labiatae (Lamiaceae), Caryophyllaceae, Fumariaceae, Violaceae, and Scrophulariaceae families better than bromoxynil. The addition of a surfactant may reduce crop selectivity.

USE PRECAUTIONS

Fire hazard: Non-flammable; in case of fire, there is risk of toxic gas fumes such as oxides of carbon, nitrogen, and iodohydric acid.
Corrosiveness: Non-corrosive to spray equipment
Storage stability: Stable in normal storage conditions; maintain above 0 C.
Cleaning glassware/spray equipment: Clean glassware with acetone; flush equipment with water.
Emergency exposure: Wash eyes with water for 20 min; wash skin with soap and water. If ingested, induce vomiting; no specific antidote is available.
Incompatibilities: Incompatible with liquid fertilizers and water-soluble 2,4-D formulations; may be incompatible with some EC formulations.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Symptoms begin within a few h with the appearance of blistered or necrotic spots on leaves of susceptible species. Chlorosis subsequently appears around the necrotic areas until the entire leaf becomes dry and necrotic, exhibiting burning symptoms.
Absorption/translocation: Absorbed readily through the cuticle (4). Selectivity is based partly on differential spray retention (7). Ioxynil esters penetrate leaves more readily than ioxynil salts. Thus, efficacy of esters is less affected by adverse environmental conditions in the field. Ioxynil is primarily a contact herbicide. Acropetal translocation of root-absorbed ioxynil is limited, as is basipetal translocation of foliar-absorbed ioxynil (4, 10).
Metabolism in plants: Little metabolism information is available. By analogy with bromoxynil, a closely related benzonitrile, ioxynil probably is metabolized by hydrolysis of the cyano group to an amide and then to a carboxylic

acid, with possible further degradation via decarboxylation, dehalogenation, and conjugation of the ring hydroxyl (2). Ioxnyil selectivity is partly attributed to differential metabolism, but may involve other factors. Liberation of iodide ions from ioxynil followed by oxidation of iodide to iodine via plant peroxidases varies with species and may be important in selectivity (9). No halogenated metabolites of ioxynil were detected in *Matricaria inodora* or *Viola arvensis* (6).

Non-herbicidal biological properties: Weak molluscidal activity, and short-lived activity against powdery mildew under some conditions.

Mechanism of resistance in weeds: No known ioxynil resistant weed populations have developed; transgenic ioxynil resistant tobacco, cotton, and canola are under investigation.

BEHAVIOR IN SOIL

Sorption: Weakly bound to soil

K_{oc}: 234 to 1420 mL/g (5)

Transformation:

Photodegradation: Negligible losses

Other degradation: Degraded microbially

Persistence: Virtually no PRE activity from normal application rates

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade ioxynil acid unless otherwise indicated.

Acute toxicity:

Oral LD$_{50}$ rat, 110 mg/kg; Dermal LD$_{50}$ rabbit, 1050 mg/kg; 4-h inhalation LC$_{50}$ rat, 0.4 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, none.

Subchronic toxicity:

90-d dietary rat: NOEL 2 mg/kg/d; liver effects

Chronic toxicity:

18-mo dietary, mouse: NOEL <1.5 mg/kg/d; liver and thyroid effects at 30 and 100 mg/kg

24-mo dietary, rat: NOEL 0.5 mg/kg/d; thyroid effects at 30 and 100 mg/kg

30-wk dietary, dog: NOEL 1 mg/kg/d; red blood cell effects (possibly reversible); excessive weight loss and anemia at 10 mg/kg/d

Teratogenicity:

Rat: NOAEL 5 mg/kg/d

Rabbit: NOAEL 15 mg/kg/d

Reproduction:

Rat: NOEL >10 mg/kg/d; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; Mouse lymphoma/forward mutation, negative.

Structural chromosome aberration: Mouse micronucleus, negative; Human lymphocyte micronucleus, negative.

DNA damage/repair: Rat hepatocyte/UDS, negative.

Wildlife:

Mallard duck oral LD$_{50}$, 1200 mg/kg; Pheasant oral LD$_{50}$, 75 mg/kg.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Phenol is reacted with acetic anhydride to produce phenyl acetate which is then brominated at the para position. Reaction with cuprous cyanide replaces the Br with a cyano group (Sandmeyer reaction). Hydrolysis of the acetate in the presence of NaOH followed by reaction with ICl in acidic conditions yields ioxynil.

Purification of technical: Ioxynil is purified by dissolving in aqueous NaOH and precipitation by acidification. Dry ioxynil can be recrystallized from hot propanol. Repeat as necessary.

Analytical methods: IR spectroscopy or GC of the methyl ester of ioxynil with an electron capture detector.

Historical: First synthesized in Germany in 1896 (1). In 1960, Amchem discovered the POST broadleaf activity of ioxynil and its selectivity in cereals. A number of ioxynil analogs including the bromo analogs appeared to have practical value. Wain (8) and Carpenter and Heywood (3) also reported the activity of ioxynil, independently of Amchem. U.S. Patent 3,397,054 covers ioxynil and bromoxynil as herbicides.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience; Adama

Reference(s):

1. Auwers and Reis. 1896. Ber. Deut. Chem. Ges. 29:2355.
2. Buckland J. L. et al. 1973. Pestic. Sci. 4:149.
3. Carpenter and Heywood. 1963. Nature 200:28-29.
4. Davies P. J. et al. 1968. Weed Res. 8:233.
5. European Commission, Health & Consumer Protection Directorate-General. 2004. Review Report for the active substance ioxynil. SANCO/4349/2000, February, 2004.
6. Moreland and Novitzky. 1984. Z. Naturforsch. 39c:329.
7. Sanders and Pallet. 1987. Pestic. Biochem. Physiol. 28:163.
8. Schaefer and Chilcote. 1970. Weed Sci. 18:729.
9. Wain, R. L. 1963. Nature 200:28.
10. Wain and Smith. 1976. Pages 279-302 *in* L. J. Audus, ed., Herbicides: Physiology, Biochemistry, Ecology, Vol. I. Academic Press, London.
11. Zaki, M. A. et al. 1961. Ann. Appl. Biol. 59:481.

isoproturon

CAS #: 34123-59-6 **7$^{(C_2)}$**

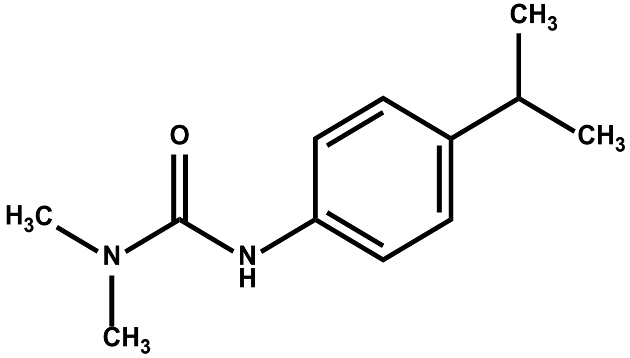
N,*N*-dimethyl-*N*′-[4-(1-methylethyl)phenyl]urea

NOMENCLATURE

Common name: isoproturon (ISO 1750 published)
Other name(s): HOE 16410; CGA-18731; 3-(4-isopropylphenyl)-1,1-dimethylurea (IUPAC); 3-*p*-cumenyl-1,1-dimethylurea (IUPAC)
Trade name(s): ALON; ARELON; GRAMINON; DFF + 1PU; TOLKAN®
Chemical family: phenylurea; substituted urea; urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
isoproturon



Molecular formula: $C_{12}H_{18}N_2O$
Molecular weight: 206.29 g/mole
Description: Colorless crystals
Density: 1.2 g/mL (20 C)
Melting point: 154 C
Boiling point: NA
Vapor pressure: 3.2 Pa (20 C); 8.1 Pa (25 C)
Stability: Very stable to light, acids, and alkalis
Solubility: (20 C): 65 mg/L; methanol 75 mg/L; dichloromethane 63 mg/L
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 2.5

HERBICIDAL USE

Isoproturon is effective against several broadleaf weeds and numerous grassy weeds (*Alopecurus myosuroides, Apera spica-venti, Avena fatua, and Poa annua*) to control in soft winter wheat, winter barley, and rye. It can be applied preemergence and postemergence.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable under normal storage conditions
Cleaning glassware/spray equipment: Wash with water and detergent
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) . (more details on page 13)
Symptomology: Injury begins as interveinal chlorosis of the leaves, followed in susceptible plants by increasing chlorosis and necrosis. Cotyledons may show chlorotic areas. Older leaves show more damage than new growth. Root growth is not affected.
Absorption/translocation: Systemic herbicide, absorbed by the roots and leaves
Metabolism in plants: Degradation is mainly via hydroxylation of the isopropyl group to 1,1-dimethyl-3-[2'-hydroxy-2'-propyl)-phenyl] urea; *N*-dealkylation also occurs.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 80 – 230 mL/g
Transformation: Isoproturon can be photodegraded, hydrolyzed, and biodegraded and persists from days to weeks. It is mobile in soil and has been detected in surface and ground water. Rate of degradation increases three fold between 10 C and 30 C (sandy soil) and 10 fold in an organic soil over the same temperature range.
Persistence: Field dissipation DT_{50} = 40 d in temperate climates; 15 d in tropical climates
Mobility: NA
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade isoproturon unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, 1826-2417 mg/kg; mice, 3350 mg/kg; Dermal LD_{50}, >2000 mg/kg; Non-irritating to skin and eyes (rabbit); 4-h inhalation LC_{50} rats, >1.95 mg/L; air, >5000 mg/kg
Subchronic toxicity:
NOEL (90 d) for rats 400 mg/kg; dogs 50 mg/kg
Chronic toxicity: (2 yr) rats 80 mg/kg
Mutagenicity: Non-mutagenic
Wildlife:
Oral LD_{50} Japanese quail, 3042-7926 mg/kg; pigeons, >5000 mg/kg; LC_{50} bluegill sunfish, >100 mg/L (96 h); LC_{50} rainbow trout, 37 mg/L (96 h); EC_{50} Daphnia magna, >507 mg/L (48 h); EC_{50} green algae, 0.03 mg/L; Oral LD_{50} >100 μg/bee
Use classification: WHO Class III

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA

Analytical methods: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience; Kwizda; Syngenta Crop Protection

Reference(s):

1. Roberts, T. 1998. Metabolic Pathways of Agrochemicals.

isoxaben

CAS #: 82558-50-7

$21^{(L)}$

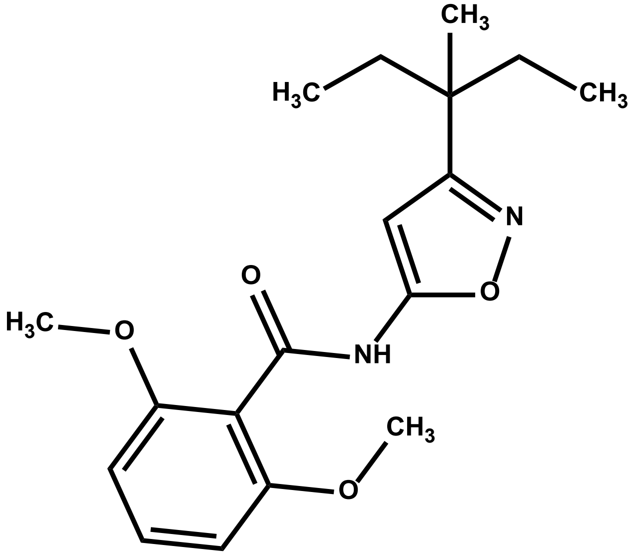
N-[3-(1-ethyl-1-methylpropyl)-5-isoxazolyl]-2,6-dimethoxybenzamide

NOMENCLATURE

Common name: isoxaben (ANSI, BSI, ISO, WSSA)
Other name(s): benzamizole; *N*-[3-(1-ethyl-1-methylpropyl)-1,2-oxazol-5-yl]-2,6-dimethoxybenzamide (IUPAC)
Trade name(s): CENT 7®; FLEXIDOR; GALLERY®; SNAPSHOT®; TRELLIS®, GALLERY SC
Chemical family: amide; benzamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
isoxaben



Molecular formula: $C_{18}H_{24}N_2O_4$
Molecular weight: 332.40 g/mole
Description: White crystalline solid
Density: 0.40-0.48 g/mL
Melting point: 176-179 C
Boiling point: NA
Vapor pressure: 5.20 x 10^{-5} Pa (26 C)
Stability: Degraded by UV light in aqueous solution; decomposes at 220 C
Solubility:
water (20 C), 1.04 mg/L un-buffered, 0.83 mg/L (pH 5), 0.93 mg/L (pH 7), and 1.83 mg/L (pH 10)
organic solvents g/100 mL:
acetone 5 (25 C) *n*-hexane 0.007 (25 C)
acetonitrile 3 (25 C) methanol 10 (20 C)
toluene 0.4 (25 C) xylene 0.4 (20 C)
ethyl acetate 9 (20 C) dichloromethane 5 (25 C)
n-octanol 2.9 (20 C) n-heptane 0.0028 (20 C)
cyclohexane 0.37 (25 C)
1,2-dichloroethane 5.1 (20 C)
pK_a: None (non-ionizable)
K_{ow}: 7780 ± 1320 (pH 5), 7870 ± 480 (pH 7), 2340 ± 115 (pH 10)

HERBICIDAL USE

Isoxaben can be applied PRE at 0.56-1.12 kg ai/ha in established turf, ornamentals, nursery stock, non-bearing fruit and nut trees, non-bearing vines, Christmas tree plantations, and non-cropland areas. Isoxaben controls bittercress, common chickweed, clover spp., dandelion, henbit, prostrate knotweed, plantain spp., spurge, and many other annual broadleaf weeds. Isoxaben activation requires a light cultivation or at least 1.3 cm of rainfall within 3 wk of application. Isoxaben is now labeled for use in bearing tree nuts and vines. Also control horseweed/marestail.

USE PRECAUTIONS

Fire hazard: GALLERY DF is dry and nonflammable; auto-ignition temperature is 415-420 C.
Corrosiveness: GALLERY, SNAPSHOT TG, and SNAPSHOT DF are non-corrosive.
Storage stability: Stable under normal storage conditions
Cleaning glassware/spray equipment: Wash with detergent and rinse with water.
Emergency exposure: If GALLERY is ingested, do not induce vomiting; administer 6-8 heaping teaspoons of activated charcoal with a large quantity of water.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits cell wall biosynthesis in susceptible weeds (2). (more details on page 15)
Symptomology: Many susceptible weeds fail to emerge following PRE- or PPI-applied isoxaben. Broadleaf weeds generally show stunting, reduced root growth, root hair distortions, and root clubbing (swelling of meristematic and elongation zones) similar to symptoms caused by dinitroaniline herbicides. Foliar application to susceptible broadleaf weeds causes growth inhibition, swelling and cracking of the stem and petiole within 2-3 d, and altered leaf hair shape in developing leaves.
Absorption/translocation: Readily absorbed into roots from soil by passive diffusion. Penetration into leaves is limited. Only 3% of foliar-applied isoxaben entered pigweed (highly susceptible) leaves by 3 d after application. Isoxaben is xylem mobile in cereals and rapeseed. Significant concentrations (>1 ppm) can accumulate in leaves within 2-3 d following root application.
Metabolism in plants: Susceptible and tolerant species metabolize up to 50% of absorbed isoxaben within 4 d following root application. Differential metabolism is not the basis of selectivity. The most abundant primary metabolite in susceptible and tolerant species is hydroxylated on the 2-carbon of the propyl side chain (both stereoisomers occur in equal abundance). Isoxaben also is hydroxylated at the propyl 3-carbon (1). More than 50% of these metabolites are then glucosylated. 2,6-dimethoxybenzamide is found as a minor metabolite. Isoxaben is readily metabolized in cereals,

primarily through hydroxylation of the alkyl side chain.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil

K_{oc}: 190-1270 mL/g

K_d: Sand 1.07 mL/g; loamy sand 2.83 mL/g; sandy loam 3.26 mL/g; clay loam 7.53 mL/g

Transformation:

Photodegradation: Based on lab photolysis half life of 60 days, very little photolysis losses would occur in the field situations.

Other degradation: Degraded slowly by microbial action under aerobic conditions to form two major metabolites. The half lives in the lab under aerobic conditions were in the range of 156-891 days. More rapid microbial degradation was observed under anaerobic condition that results in four different major metabolites in the total system. The half lives in the lab under anaerobic conditions were in the range of 3-71 days in the total system.

Persistence: Moderately persistent with a calculated field geometric mean DT_{50} of 94.3 days. Effective weed control usually extends 5-6 months at labeled rates.

Mobility: Leaches slightly in laboratory soil columns and in the field.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade isoxaben unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat and mouse, >10,000 mg/kg; dog, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >2.68 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, mouse: NOEL 15.5 mg/kg/d

90-d dietary, rat: NOEL 9 mg/kg/d

90-d dietary, dog: NOEL 110 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL NA; minor hepatotoxic effects at ~118 mg/kg/d; benign proliferative hepatocellular lesions at ~1522 mg/kg/d; not carcinogenic; a Class C oncogen

24-mo dietary, rat: NOEL NA; no cumulative toxicity or serious adverse effects at up to ~57 mg/kg/d; chronic nephrotoxic effects at ~587 mg/kg/d; not carcinogenic or oncogenic

12-mo dietary, dog: NOEL 10 mg/kg/d; minor liver effects at 100 mg/kg/d

Teratogenicity:

Rat: NOEL NA; not teratogenic at 330 mg/kg/d

Rabbit: NOEL NA; not teratogenic at 1000 mg/kg/d

Reproduction:

Rat: NOEL NA; fetal malformation in 17 of 139 litters with indications of toxicity in parents of both sexes at 1000 mg/kg/d (not clear whether these abnormalities resulted from isoxaben-induced maternal toxicity, a direct teratogenic effect, or an interaction of genetic and environmental factors); no fetal toxicity at 200 mg/kg/d.

Mutagenicity:

Structural chromosome aberration: Mouse micronucleus, positive (Class C oncogen based on increases in liver adenomas in mice and positive micronucleus test).

Wildlife:

Bobwhite quail oral LD50, >2000 mg/kg body weight, 8-d dietary LC50, >5000 mg/kg diet; Mallard duck oral LD50, >5000 mg/kg, 8-d dietary LC50, >5000 mg/kg diet; Earthworm LC50 in soil, >100 mg/kg soil; Honey bee topical LD50, >100 µg/bee; Daphnia 48-h LC50, >1.3 mg/L; Bluegill sunfish 96-h LC50, >1.1 mg/L; Rainbow trout 96-h LC50, >1.1 mg/L; Green algae 14-d EC50, >1.4 mg/L; Duckweed 14-d EC50 = 0.013 mg/L.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Formulated products are dissolved in or extracted with methanol and the resulting solution analyzed by HPLC with UV detection at 254 nm. Residue determination requires extraction of crop tissue or soil with methanol, removal of interfering substances with solvent partitioning and alumina column chromatography, and determination by HPLC with UV detection at 254 nm. Assay sensitivity is approximately 10 mg/kg.

Historical: Discovered in 1979; first reported in 1982 (3); introduced in France in 1984 by Eli Lilly & Company; British patent 2,084,140

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

Reference(s):

1. Corio-Costet, M.-F. et al. 1991. Pestic. Biochem. Physiol. 40:246.
2. Heim, D. R. et al. 1990. Plant Physiol. 93:695.
3. Huggenberger, F. et al. 1982. Proc. Br. Crop Prot. Conf.-Weeds 1:47.

isoxaflutole

CAS #: 141112-29-0

$27^{(F_2)}$

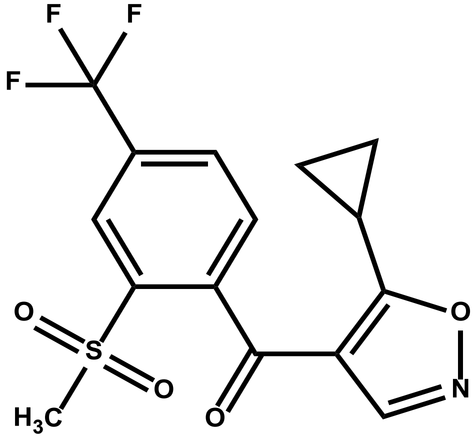
(5-cyclopropyl-4-isoxazolyl)[2-(methysulfonyl)-4-(trifluoromethyl)phenyl]methanone

NOMENCLATURE

Common name: isoxaflutole
Other name(s): RP-201772; 5-cyclopropyl-1,2-oxazol-4-yl) (α,α,α-trifluoro-2-mesyl-*p*-tolyl ketone (IUPAC)
Trade name(s): ATOLL®; BALANCE®; BOREAL®; LAGON®; MERLIN®; PROVENCE®
Chemical family: cyclopropylisoxazole; isoxazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *isoxaflutole*



Molecular formula: $C_{15}H_{12}F_3NO_4S$
Molecular weight: 359.32 g/mole
Description: Off-white/pale yellow solid
Density: 1590 g/L
Melting point: 140 C
Boiling point: NA
Vapor pressure: 3.2×10^{-7} Pa (20 C); 1×10^{-6} Pa (25 C); Henry's Law constant, 1.87×10^{-5} Pa m^3 mol^{-1}
Stability: Stable
Solubility:

water, 6.8 mg/L (pH 5); 6.2 mg/L (pH 5.5); decomposes at pH 9
organic solvents (g/L) (20 C):
hexane 0.10
dichloromethane 346
acetone 293
methanol 13.8
acetonitrile 233
ethyl acetate 142
toluene 31.2
octanol 0.76

pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 2.32

HERBICIDAL USE

Isoxaflutole can be applied PRE or early preplant at 75 to 140 g ai/ha for the control of broadleaf and grass weeds in corn and sugarcane. Susceptible weeds include velvetleaf, common ragweed, common lambsquarters, redroot pigweed, smooth pigweed, kochia, Pennsylvania smartweed, fall panicum, wild proso millet, barnyardgrass, and foxtails (giant, green, and yellow).

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: Non-corrosive
Storage stability: Stable under normal storage conditions
Cleaning glassware/spray equipment: Wash with water and detergent
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme 4-hydroxyphenyl-pyruvate dioxygenase (4-HPPD) affecting carotenoid biosynthesis. (more details on page 15)
Symptomology: Major symptoms include bleaching of new growth
Absorption/translocation: Primarily in the xylem
Metabolism in plants: The tolerance of corn to isoxaflutole is due to rapid metabolism via hydrolytic reactions, which are poorly understood at the present time. Sensitive weeds metabolize the herbicide at a much slower rate.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Some weed biotypes may have altered target sites.

BEHAVIOR IN SOIL

Sorption: K_{oc} ranges from 93to 131 mL/g; mean 112 mL/g (technical)
Transformation: Isoxaflutole is degraded via chemical hydrolysis and soil microbial action.

Photolytic degradation: DT_{50} (pH 5, 25 C), 40 h
Other degradation: Laboratory degradation DT_{50} ranged from 0.5 to 4 d (20 C); field dissipation DT_{50} ranged from 0.5 to 2.4 d

Mobility: Laboratory studies indicate that under simulated high rainfall conditions, isoxaflutole and its metabolites could be soil mobile
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade isoxaflutole unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.3 mg/L (max. attainable conc.); Skin irritation rabbit, no; Skin sensitization guinea pig, no; Eye irritation rabbit, no

Subchronic toxicity:

90-d dietary, mice: NOEL 1002 mg/kg/d (6400 mg/kg) for males; 1178 mg/kg/d for females

Mutagenicity:

Gene mutation: CHO/HGPRT, negative
Structural chromosome aberration: CHO, negative; Rat bone marrow, negative

DNA damage/repair: Primary rat hepato-cytes/UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; Daphnia 48-h EC_{50}, non-toxic; Bluegill sunfish 96-h LC_{50}, non-toxic; Rainbow trout 96-h LC_{50}, non-toxic

Use classification: Restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purfication of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Luscombe, B.M. et al. 1995. Proc. Brighton Crop Prot. Conf. – Weeds. Pp. 35-42.
2. European Commission Health & Consumer Protection Directorate-General. 2003. Isoxaflutole, SANO/3136/99-Final, April 7, 2003.

lactofen

CAS #: 77501-63-4

$14^{(E)}$

2-ethoxy-1-methyl-2-oxoethyl 5-[2-chloro-4-(trifluoromethyl) phenoxy]-2-nitrobenzoate

NOMENCLATURE

Common name: lactofen (ANSI, WSSA)

Other name(s): PPG-844; ethyl *O*-[5-(2-chloro-α,α,α-trifluoro-*p*-tolyloxy)-2-nitrobenzoyl]-*DL*-lactate (IUPAC)

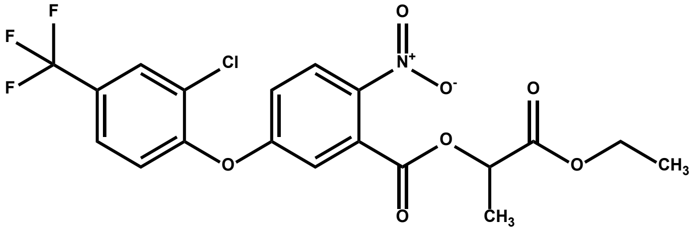
Trade name(s): COBRA®

Chemical family: diphenylether; nitrodiphenylether; nitrophenylether

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

lactofen



Molecular formula: $C_{19}H_{15}ClF_3NO_7$

Molecular weight: 461.78 g/mole

Description: White crystalline solid (when pure), faint aromatic odor

Density: 1.39 g/mL (25 C)

Melting point: 43.9 - 45.5 C

Boiling point: NA

Vapor pressure: 5.3×10^{-7} Pa (20 C); 1×10^{-6} Pa (25 C)

Stability: Decomposes at 275 C; unstable at pH 9

Solubility:

- water 0.1 mg/L (22 C)
- organic solvents g/100 mL (25 C)
- acetone miscible (≥-18 C)
- 2-propanol 1.92 (4 C)
- isopropanol 20
- xylene miscible (≥-18 C)
- kerosene 1.27 (23 C)

pK_a: None (non-ionizable)

K_{ow}: NA

HERBICIDAL USE

Lactofen can be applied POST at 0.07-0.22 kg ai/ha in soybeans, POST-directed at 0.22 kg ai/ha in cotton, and POST at 0.11-0.22 kg ai/ha in southern pine seedlings. It controls many annual broadleaf weeds such as jimsonweed, wild mustard, nightshade spp., ragweed spp., pigweed spp., and cocklebur. Oil adjuvants, surfactants, and fertilizer adjuvants often are added to enhance control.

USE PRECAUTIONS

Fire hazard: COBRA is combustible; flash point is 40 C.

Corrosiveness: COBRA is non-corrosive to mild steel or other materials normally used in spray equipment.

Storage stability: COBRA does not freeze above 0 C. Cobra had excellent stability in 2-yr tests conducted over a range of normal storage conditions.

Cleaning glassware/spray equipment: Rinse equipment with water

Emergency exposure: If ingested, do not induce vomiting; drink large quantities of milk, egg whites, gelatin solution, or, if these are not available, water; consult a physician.

Incompatibilities: No known incompatibilities with other herbicides or liquid fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)

Symptomology: Leaves of susceptible plants become chlorotic and then desiccated and necrotic within 1-2 d. Youngest expanded leaves of soybeans also may show chlorosis and necrosis, especially at higher rates. Sublethal rates may produce foliar bronzing, usually on young expanded leaves or on needles of pine seedlings. Droplet drift may cause bleached spots or flecks on leaves.

Absorption/translocation: Readily absorbed by leaves of most species. Very little foliar-absorbed lactofen translocates basipetally. Absorption by roots and acropetal translocation to leaves also are limited.

Metabolism in plants: Readily metabolized by plants; no measurable residues have been detected longer than 24 d after treatment

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Resistance to PPO inhibitors is due to a deletion in the PPO gene.

BEHAVIOR IN SOIL

Sorption: Strongly absorbed to OM

K_{oc}: Average is 10,000 mL/g (estimated) (3)

Transformation:

Photodegradation: Half-life was 23 d. Photodegradation losses probably do not contribute greatly to field dissipation because of rapid breakdown by microbes.

Other degradation: Degrades quickly under aerobic conditions, but more slowly in anaerobic conditions. Lactofen is rapidly hydrolyzed in water at pH but is stable at pH values of 5 and 7. Non-microbial degradation appears to be insignificant.

Persistence: Average field half-life is 3 d (3). Lactofen usually dissipates in ≤7 d in most soils. Soil activity sometimes lasts for 2-3 wk on sensitive species. Residues do not injure rotational crops planted the following season.

Mobility: Immobile in soil. Degradation products of lactofen are highly mobile in sandy soil and have low to moderate mobility in soil with high OM and clay contents.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade lactofen unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 5960 mg/kg; Dermal LD_{50} rabbit, > 2000 mg/kg; 4-h inhalation LC_{50} rat, >3.6 mg/L; Skin irritation rabbit, slight; Skin sensitize guinea pig, no; Eye irritation, NA

COBRA: Oral LD_{50} rat, 2533 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 6650 mg/L; Eye irritation rabbit, severe

Subchronic toxicity:

90-d dietary, rat: NOEL 10 mg/kg/d (200 mg/kg), LOEL 50 mg/kg/d (1000 mg/kg)

Chronic toxicity:

18-mo dietary, mouse: LOEL 1.5 mg/kg/d (10 mg/kg); increased liver weight and hepatocylomegally; increased combined incidence of liver adenomas and carcinomas at 250 mg/kg

24-mo dietary, rat*:* Systemic NOEL 25 mg/kg/d (500 mg/kg), LOEL 50 mg/kg/d (1000 mg/kg); kidney and liver pigmentations; increased incidence of liver neoplastic nodules and foci of cellular alteration of 2000 mg/kg

12-mo dietary dog: NOEL 5 mg/kg/d (200 mg/kg), LOEL 25/75 mg/kg/d (1000/3000 mg/kg); renal dysfunction, and increased Hgb, Hct, red blood cells, and cholesterol

Teratogenicity:

Rat: NOEL 50 mg/kg/d, LOEL 150 mg/kg/d; maternal post implantation loss and reduced body weight, fetal bent ribs; not teratogenic

Rabbit: NOEL 4 mg/kg/d, LOEL 20 mg/kg/d; reduced maternal food consumption; not teratogenic

Reproduction:

Rat: NOEL 2.5 mg/kg/d (50 mg/kg), LOEL 25 mg/kg/d (500 mg/kg); reduced mean pup weight; increased pup heart and liver weight

Mutagenicity:

Gene mutation: Ames test, negative in Study 1, positive in Study 2

Structural chromosome aberration: Unspecified test, negative

DNA damage/repair: Unspecified test, negative; UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2510 mg/kg, 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary $LC_{50,}$ >5620 mg/kg; Honey bee topical LD_{50}, >160 μg/bee; Daphnia 48-h LC_{50}, 2 mg/L; Bluegill sunfish 96-h LC_{50}, >560 mg/L; Rainbow trout 96-h LC_{50}, >0.1 mg/L

COBRA: Daphnia 48-h LC_{50}, 5.1 mg/L; Bluegill sunfish 96-h LC_{50}, 0.49 mg/L; Rainbow trout 96-h LC_{50}, 0.85 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: See the “Pesticide Analytical Manual” published by the Food and Drug Administration.

Historical: Introduced by PPG Industries

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Valent

Reference(s):

1. Duke, S. O. et al. 1991. Weed Sci. 39:465.
2. Lee and Duke; 1994. Abstr. Weed Sci. Soc. Am. 34:52.
3. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

linuron

CAS #: 330-55-2 $7^{(C_2)}$

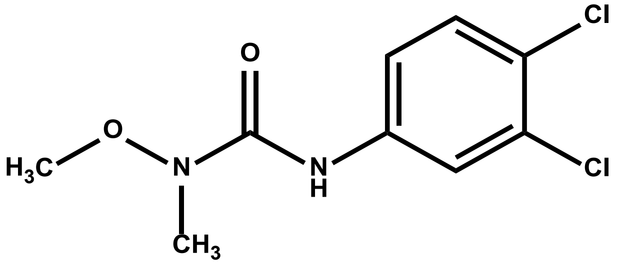
N′-(3,4-dichlorophenyl)-*N*-methoxy-*N*-methylurea

NOMENCLATURE

Common name: linuron (ANSI, BSI, ISO, WSSA)
Other name(s): DUPONT HERBICIDE 326; HOE 2810; 3-(3,4-dichlorophenyl)-1-methoxy-1-methyl-urea (IUPAC)
Trade name(s): ALIBI FL; LAYBY™ PRO; LINEX®; LINEX 4L; LINOROX; LOROX®; LOROX® DF; MALURANE; POTABLAN S; PREMALIN; SARCLEX; SUPER PKW
Chemical family: phenylurea; substituted urea; urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
linuron



Molecular formula: $C_9H_{10}Cl_2N_2O_2$
Molecular weight: 249.10 g/mole
Description: White crystalline solid, odorless
Density: NA
Melting point: 93-94 C
Boiling point: NA
Vapor pressure: 51 Pa (20 C)
Stability: Stable at 93-94 C
Solubility:
water 75 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 50
benzene 15
ethanol 15
heptane 1.5
xylene 13
pK_a: None (non-ionizable)
K_{ow}: 1010

HERBICIDAL USE

Linuron can be applied as follows: PRE at 0.37-2.8 kg ai/ha or directed-POST at 0.28-1.12 kg ai/ha in soy-beans; PRE at 0.37-1.68 kg ai/ha or directed POST at 0.7-1.68 kg ai/ha in corn; PRE at 1.12-2.24 kg ai/ha (with activated charcoal over the row) or POST at 0.56-1.12 kg ai/ha in new plantings of asparagus; PRE at 1.12-2.24 kg ai/ha, POST at 0.56-1.12 kg ai/ha, or directed-POST at 2.24-4.5 kg ai/ha in established asparagus; PRE at 0.56-1.7 kg ai/ha or POST at 0.84-1.7 kg ai/ha in carrots; POST at 0.84-1.7 kg ai/ha in celery; at 1.12-2.24 kg ai/ha before bud break in hybrid poplar or as a directed spray at 1.12-2.24 kg ai/ha after bud break; PRE at 0.84-1.7 kg ai/ha in parsnips; PRE at 0.56-2.24 kg ai/ha in potatoes; and PRE at 0.35-1.12 kg ai/ha or directed-POST at 0.56-1.12 kg ai/ha in sorghum. Linuron controls annual broadleaf weeds, including mustard spp., pigweed spp., Florida pusley, purslane, and Pennsylvania smartweed, and certain annual grasses such as barnyardgrass and foxtail spp. Foliar applications are effective on a wider spectrum of weeds. A non-ionic surfactant increases the efficacy of applications to weed foliage. Linuron may be applied in liquid fertilizer.

USE PRECAUTIONS

Fire hazard: All formulated products are dry or aqueous and non-flammable.
Corrosiveness: Non-corrosive
Storage stability: Dry formulations are stable under normal storage conditions.
Cleaning glassware/spray equipment: Flush sprayer with water after removing nozzle tips and screens (clean tips and screens separately); clean glassware by detergent wash followed by acetone rinse
Emergency exposure: May irritate eyes, nose, throat, and skin
Incompatibilities: All formulated products are compatible with most other herbicides with which they might be mixed. Certain ester formulations of hormone herbicides may create a physical problem in the spray tank.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: With soil applications, seedlings emerge but become chlorotic within a few days, followed by complete necrosis. Foliar applications begin with interveinal chlorosis of the leaves and yellowing of their margins. Further chlorosis and necrosis follows in susceptible plants. Older leaves are more damaged than new growth.
Absorption/translocation: Absorbed readily into roots following soil application, but less so into leaves and stems when foliar-applied; however, foliar absorption of linuron is significantly greater than that of diuron, monuron, or fenuron (6); linuron readily translocates acropetally in the xylem with little to no basipetal movement in the phloem
Metabolism in plants: Several plant species oxidatively *N*-dealkylate linuron (5). Linuron was oxidized by inducible monooxygenases in wheat (3).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Linuron resistance was found in redroot pigweed and horseweed in Hungary (7).

BEHAVIOR IN SOIL

Sorption: Adsorption increases as soil clay or OM content increases. More linuron is adsorbed by soils of high than of low cation exchange capacity. Linuron has about the same tendency for adsorption as diuron. For example, 5.5 mg/kg of linuron is adsorbed on Keyport silt loam in equilibrium with

1 mg/kg in soil solution at 22 C, compared with 5.2 mg/kg of diuron.

K_{oc}: Average is 400 mL/g (9)

Transformation:

Photodegradation: Probably insignificant losses except where soil is warm and no activating rainfall is received for several days or weeks after application, leaving linuron on the soil surface

Other degradation: Microbial breakdown is the primary means of linuron dissipation from soil (2).

Persistence: Average field half-life is 60 d (9), but ranges from 2-5 mo; linuron residues from spring applications do not injure cover crops planted the following fall

Field experiments: Oat bioassays have indicated no phytotoxic soil residues 3-4 mo after application at selective rates.

Mobility: Leaching probably is not an important factor in dissipation from most soils. Linuron leaches most in sand and least in soils high in clay or OM

Volatilization: Probably insignificant losses except where soil is warm and no activating rainfall is received for several days or weeks after application, leaving linuron on the soil surface

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade linuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 1254 mg/kg; female rat, 1196 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, 6.15 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, mild

Subchronic toxicity:90-d dietary, rat: NOEL male 80 mg/kg

Chronic toxicity:

24-mo dietary, mouse: NOEL 150 mg/kg; hepatocellular adenoma in females at 1500 mg/kg.

24-mo dietary, rat: NOEL 50 mg/kg; red blood cell effects at all levels; testicular interstitial cell adenomas at 125 mg/kg

24-mo dietary, dog: NOEL 25 mg/kg; anemia

Teratogenicity:

Rat: NOEL 125 mg/kg; not teratogenic; weight gain

Rabbit: NOEL maternal 5 mg/kg/d, fetus 25 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 25 mg/kg in a 3-generation study

Mutagenicity:

Gene mutation: Ames test, negative; *E. coli*, negative; CHO, negative

Structural chromosome aberration: *In vivo* cytogenetics, negative

Wildlife:

Japanese quail 8-d LC_{50}, >5000 mg/kg; Mallard duck 8-d dietary LC_{50}, 3083 mg/kg; Ring-necked pheasant 8-d dietary LC_{50}, 3438 mg/kg; Bluegill sunfish 96-h LC_{50}, 16 mg/L; Carp 48-h TLM, 7 mg/L; Rainbow trout 96-h LC_{50}, 16 mg/L; Crawfish 72-h TLM, >40 mg/L; Tadpole 48-h TLM, >40 mg/L

Use classification: General use.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React 3,4-dichlorophenyl-isocyanate with methoxymethylamine (dimethyl hydroxylamine)

Purification of technical: Recrystallize twice from absolute ethanol or 95% ethanol

Analytical methods: Residues are determined by quantitative hydrolysis of linuron under reflux conditions in a strongly alkaline medium. The resulting aromatic amine is separated and determined colorimetrically after diazotization and coupling reactions. Interfering compounds are eliminated by chromatography (1, 8).

Historical: First reported in 1962 (4); introduced by Du Pont Company and by Hoechst AG. German patent 1,028.986 and British patent 852,422 were issued to Hoechst AG

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama, DuPont Crop Protection; Drexel; Griffin;

Reference(s):

1. Dalton and Pease. 1962. J. Assoc. Offic. Anal. Chem. 45:377.
2. Dubrey and Freeman. 1964. Soil Sci. 97:334.
3. Frear, D. S. et al. 1991. Pestic. Biochem. Physiol. 41:274.
4. Hartel, K. 1962. Meded. Landbouwhogesch. Opzoekingsstn. Staat Gent. 27:1275.
5. Hatzios, K. K. and D. Penner. 1982. Metabolism of Herbicides in Higher Plants. Burgess Publ. Co., Minneapolis.
6. Hill, G. D. et al. 1962. Proc. Northeast. Weed Control Conf. 16:348.7. LeBaron, H. M. 1991. Pages 27-66 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Ltd., Oxford.
8. Pease, H. L. 1962. J. Agric. Food Chem. 10:279.
9. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

maleic hydrazide

1,2-dihydro-3,6-pyridazinedione

CAS # Acid: 123-33-1
Potassium salt: 28382-15-2

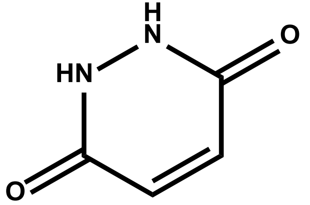
NC

NOMENCLATURE

Common name: maleic hydrazide (BSI, ISO, WSSA)
Other name(s): 6-hydroxy-2*H*-pyridazin-3-one (IUPAC); 1,2-dihydropyridazine-3,6-dione (IUPAC)
Trade name(s): MALEIC HYDRAZIDE; ROYAL MH-30®; ROYAL MH-30 XTRA; ROYAL SLO GRO
SUCKER STUFF; SPROUT STOP; SUPER SUCKER STUFF
Chemical family: None generally accepted

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
maleic hydrazide



Molecular formula: *Acid:* $C_4H_4N_2O_2$: *K salt:* $C_4H_3KN_2O_2$
Molecular weight: *Acid:* 112.09 g/mole; *K salt:* 150.18 g/mole
Description: White solid, odorless
Density: 1.60 g/mL
Melting point: 300 C
Boiling point: Decomposes before boiling
Vapor pressure: 9.99×10^{-6} Pa (25 C); Henry's Law constant, 2.5×10^{-5} Pa m^3/mole (pH 7, 25 C)
Stability: Stable to UV light; decomposes at ~260 C
Solubility:

Acid
water 4500 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C):
acetone 0.1
dimethylformamide 2.04
DMSO 9
ethanol 0.1
n-hexane <0.0001
methanol 0.418
toluene <0.0001
xylene <0.1

Potassium salt
Water 300,000 mg/L (20 C); 340,000 mg/L (25 C)

pK_a: 5.62 (20 C)**K_{ow}:** 0.21 (pH 5), 0.011 (pH 7), and 0.00385 (pH 9)

HERBICIDAL USE

Maleic hydrazide can be used for sprout control in onions and potatoes, to reduce volunteer potato growth in the year following potato production, or to retard sucker development in tobacco. It can be applied at 2.18 kg ae/ha 10-14 d before harvest in onions, at 3.36 kg ae/ha in late flowering of potatoes, at 2.5-5 kg ae/ha in full flowering of tobacco.

USE PRECAUTIONS

Fire hazard: All formulated products are dry or aqueous and are nonflammable.
Corrosiveness: Liquid formulated products are corrosive to brass nozzles if sprayed undiluted.
Storage stability: Formulated products are stable for >10 yr. Good light and temperature stability.
Cleaning glassware/spray equipment: Wash and rinse equipment with water.
Emergency exposure: If ingested, drink 1-2 glasses of water and induce vomiting.
Incompatibilities: Maleic hydrazide acid may precipitate at low pH.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Maleic hydrazide may act as a uracil anti-metabolite.
Symptomology: NA
Absorption/translocation: Slowly absorbed over a period of 24 h by quackgrass. Rain within this period reduces efficacy. Most effective absorption occurs when soil moisture is at field capacity and relative humidity is high. Foliar-absorbed maleic hydrazide translocates basipetally with accumulation at the growing points. Acropetal translocation is slower.
Metabolism in plants: Maleic hydrazide does not appear to be metabolized appreciably.
Non-herbicidal biological properties: Mildly fungicidal (1)
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Binds to soil rapidly and with moderate strength.
K_{oc}: Average is 20 mL/g (estimated) for the K salt form (2) and 250 mL/g (estimated) for the acid (3). K_{oc} was 264 mL/g for clay and 23 mL/g for sand
Transformation: Rapidly degraded by microbes. Half-life was 11 h under aerobic laboratory conditions.
Persistence: Average field half-life is estimated at 30 d (2). Residues do not injure rotational crops planted the following season.
Field experiments: Half-lives were as follows: 2-3 d in a sandy loam (potatoes); 6 d in a sandy loam (turf); 7 d in a loam (tobacco)
Mobility: Moderately mobile, but rapid degradation in soil prevents leaching under most conditions.
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade maleic hydrazide acid unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50}, NA;
Skin irritation rabbit, slight; Skin sensitization, NA; Eye irritation rabbit, slight

Maleic hydrazide Potassium salt technical: 4-h inhalation LC_{50} rat, 4.03 mg/L; Skin sensitization guinea pig, no

ROYAL MH-30: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50} rat, >20 mg/L; Skin irritation rabbit, slight; Eye irritation rabbit, slight

ROYAL MH-30 SG: Oral LD_{50} rat, 7500 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, slight; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, rat: NOEL 50 mg/kg/d

90-d dietary, dog: NOEL 1250 mg/kg/d

Chronic toxicity:

24-mo dietary, mouse: NOEL >1429 mg/kg/d; not carcinogenic

24-mo dietary, rat: NOEL 25 mg/kg/d; not carcinogenic

12-mo dietary, dog: NOEL 18.75 mg/kg/d

Teratogenicity:

Rat: NOEL >1000 mg/kg/d; not teratogenic

Rabbit: NOEL >1000 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 500 mg/kg/d; no reproductive effects

Mutagenicity:

Gene mutation: Ames test, negative; Mouse lymphoma, negative

Structural chromosome aberration: Mouse micronucleus, negative; CHO/chromosome aberration, equivocal; CHO/SCE, positive; Mouse bone marrow/ SCE, negative

DNA damage/repair: *E. coli*, negative; *B. subtilis* Rec assay, positive

Wildlife:

Mallard duck oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50} >10,000 mg/kg; Daphnia 48-h LC_{50}, 108 mg/L; Bluegill sunfish 96-h LC_{50}, 354 mg/L; Rainbow trout 96-h LC_{50}, >1435 mg/L

Maleic hydrazide Potassium salt technical: Mallard duck oral LD_{50}, >4640 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Honey bee oral LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >1000 mg/L; Bluegill sunfish 96-h LC_{50}, 1608 mg/L; Rainbow trout 96-h LC_{50}, >1000 mg/L; Algae 5-d IC_{50}, >10 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Maleic anhydride is reacted with a mineral acid or organic acid salt of hydrazine in water. The product is filtered and washed free of impurities.

Purification of technical: Water washing until a pH of approximately 2.2 is obtained.

Analytical methods: Product analysis by HPLC. Residues are determined by hydrolysis to hydrazine which is determined by colorimetry.

Historical: Synthesized and herbicidal properties discovered in 1947. Plant growth regulating properties first reported in 1949 (4). Introduced by U.S. Rubber Co.; U.S. patents 2,575,954, 2,614,912, 2,614,917, and 2,805,926.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Drexel; UAP-Platte; Uniroyal; UAP-Loveland Products

Reference(s):

1. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
2. Zukel, J. W. 1954. Agric. Chem. 9:46,113.
3. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1..
4. Schoene and Hoffman. 1949. Science 109:588.
5. Weller, L.E., C.D. Ball, H.M. Sell. 1957. Plant Phys. 32:146-148.

MCPA

CAS # Acid: 94-74-6 **4$^{(O)}$**

(4-chloro-2-methylphenoxy)acetic acid

NOMENCLATURE

Common name: MCPA (BSI, ISO, WSSA)

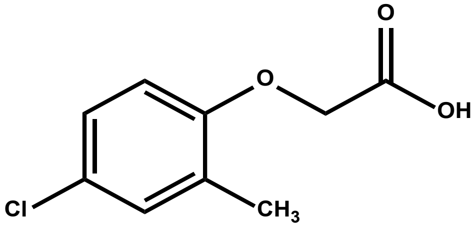
Other name(s): metaxon; 2-methyl-4-chlorophenoxyacetic acid; 4-chloro-2-methylphenoxyacetic acid; [(4-chloro-o-tolyl)oxy]acetic acid; 4-chloro-o-tolyloxyacetic acid (IUPAC)

Trade name(s): AGROXONE; BANLENE PLUS; BATTLESHIP; BISON®; BLESAL MC; BORDERMASTER; BRONATE®; BRONATE® ADVANCED; CAMBILENE; CEKHERBEX; CORNOX PLUS; CHIPTOX®; CLASS® MCPA™; CLASS MCPE™; CLEARMAX; CHEYENNE®; CURTAIL™; DAKOTA®; DED-WEED; HORMOTUHO; KILSEM; LEGUMEX EXTRA; MEPHANAC; METAXON; MIDOX FORTE; MCP AMINE; MCP 2 SODIUM; BRONATE®; MCPA-2 AMINE; MCPA LOW VOLATILE ESTER; MCPA AMINE; MCPA LV ESTER; MAYCLENE; MCP; 2,4-MCPA; 2M-4Kh; RHOMEME®; RHONOX®; MXL™ HERBICIDE; SHAMROX; STARANE® + SWORD®; SWORD®; TILLER®; ENCORE® DSC; TRIMEC® ENCORE; TRIAMINE™ II; TRI-ESTER™ II; TRIPOWER®; TRIPOWER® DRY; VACATE; VETERAN™ 2010; WEEDRHAP; WILDCARD™; WILDCARDTM XTRA; ZELAN

Chemical family: phenoxy, phenoxyacetic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: MCPA acid



Molecular formula: Acid $C_9H_9ClO_3$; Dimethylamine (Dma) salt $C_{11}H_{16}ClNO_3$; Isooctyl ester (Io ester) $C_{17}H_{25}ClO_3$

Molecular weight: Acid 200.62 g/mole; Dma salt 245.71 g/mole; Io ester 312.84 g/mole

Description: Technical is a light brown solid; pure is a colorless crystalline solid

Density: 1.56 g/mL (25/15.5 C)

Melting point: 118-119 C (pure); 99-107 C (technical)

Boiling point: NA

Vapor pressure: Acid 2.0 x 10^{-4} Pa (20 C); Dma salt negligible

Stability: NA

Solubility:

Acid

water 825 mg/L (25 C)

organic solvents g/100 mL:

ether 77	toluene 6.2
ethanol 153	xylene 4.9
n-heptane 0.5	

benzene essentially insoluble

Dimethylamine salt

water 866,000 mg/L (pH 7) (10)

Isooctyl ester

water 5 mg/L (estimated) (25 C) (10)

Sodium salt

water 270,000 mg/L (25 C)

pK_a: 3.12 (weak acid)

K_{ow}: NA

HERBICIDAL USE

MCPA can be applied as follows: POST at 0.26-1.7 kg ae/ha in wheat, barley, oats, and rye; POST at 0.13-0.28 kg ae/ha in flax; POST at 0.78-1.4 kg ae/ha in rice; POST at 0.28-0.42 kg ae/ha in peas; POST at 0.52-1.55 kg ae/ha in established rangeland and established turf; and POST at 0.52-1.04 kg ae/ha in grasses grown for seed production. MCPA controls several annual broadleaf weeds such as pigweed spp., cocklebur, ragweed spp., shepherd's-purse, and dandelion.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: Non-corrosive

Storage stability: Amine salts are stable indefinitely. Ester shelf life varies with formulation.

Cleaning glassware/spray equipment: Wash with detergent and rinse with water. Sprayers should not be used on sensitive crops until fully decontaminated. Small amounts of residues in spray equipment can be redissolved into the next load and may cause injury if applied POST to sensitive broadleaf crops.

Emergency exposure: If ingested, give plenty of water and induce vomiting.

Incompatibilities: Usually compatible

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood but similar to that of endogenous auxin (IAA) (more details on page 12)

Symptomology: Symptoms include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 3-5 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.

Absorption: Readily absorbed into leaves. Absorption is increased by wetting agents. MCPA can be washed off the leaf surface by rain soon after application. Foliar penetration of MCPA is more rapid than that of MCPB (apparently because of greater partitioning of MCPB into wax), and this may account for greater susceptibility of broad bean (Vicia faba) to MCPA (4). MCPA esters penetrate cuticles more rapidly than amine formulations. MCPA applied as a salt is protonated in the acidic environment outside the plasmalemma, and readily penetrates the plasmalemma as the protonated acid. Once inside the cell, the more-alkaline cytoplasm causes dissociation to produce MCPA anion which is trapped inside the cell due to its reduced ability to traverse the plasmalemma. Residues on the soil surface can be washed into the soil by rain occurring soon after application and are readily absorbed by roots and emerging shoots.

Translocation: MCPA is among the more mobile phenoxy herbicides. It is transported in plant tissues primarily via the symplastic pathway (including the phloem) and accumulates at the growing points. Translocation rate in tolerant species appears to be slower, perhaps because of formation of immobile complexes, reduced xylem transport, and anatomical differences among species (1).

Metabolism in plants: MCPA esters are hydrolyzed rapidly to yield MCPA acid. Subsequently, the 2-methyl group is hydroxylated to form (4-chloro-2-hydroxymethylphenoxy)acetic acid which then can be conjugated to glucose. Formation of the glucose ester of MCPA also has been reported, as well as conjugates with aspartic acid and perhaps other amino acids (1). Similar metabolites were identified in callus cells of wheat (2). After 24 h, the primary metabolite (49%) was the glycoside of (4-chloro-2-hydroxymethylphenoxy)acetic acid with very little unmetabolized MCPA remaining.

Non-herbicidal biological properties: MCPA retards tiller development in winter wheat when applied in the fall (5). Total spike number was reduced, but tiller synchrony was improved and kernel number increased on the primary spike.

Mechanism of resistance in weeds: Mecoprop and MCPA resistance in a biotype of common chickweed has occurred in Britain (6). The mechanism of resistance appears to involve rapid herbicide metabolism and subsequent formation of non-herbicidal conjugates (3). A biotype of wild mustard from Western Canada is resistant to MCPA and other auxin-mimicking herbicides. Although the mechanism of resistance is unknown, much of the evidence suggests an insensitive herbicide binding site (7, 11).

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 110 mL/g for the acid, 1000 mL/g (estimated) for the butoxyethyl and isooctyl esters, and 20 mL/g (estimated) for the dimethylamine salt (10)

Transformation:

Photodegradation: Relatively stable to light

Other degradation: Probably metabolized microbially by hydroxylation and by cleavage of the ether linkage.

Persistence: Typical half-life is 5-6 d. Persists up to 1 mo in moist conditions and up to 6 mo under drier conditions.

Mobility: Readily leached from soil

Volatilization: Minor losses with salt formulations

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade MCPA acid unless otherwise indicated.

Acute toxicity:

Oral LD50 rat, 1160, mouse 800 mg/kg; Dermal LD50 rabbit, >4000 mg/kg; 4-h inhalation LC50, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

Subchronic toxicity:

2-mo dietary, rat: NOEL NA; reduced weight gain at 100 mg/kg/d

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail oral LD50, 377 mg/kg; Honey bee oral LD50, 104 µg/bee; Rainbow trout 96-h LC50, 117 mg/L

Use classification: BRONATE is Restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Chlorination of o-cresol to produce p-chloro-o-cresol followed by coupling with mono-chloroacetic acid in an alkaline medium

Purification of technical: NA

Analytical methods: GC methods are available on request. Residue methods can be found in PAM. 1974. Vol. II. Sec. 180.339.

Historical: One of the first hormone-type herbicides discovered in England. Its plant-growth regulating activity was first reported in 1945 (8). Introduced as a herbicide by ICI Plant Protection Division and subsequently by many other companies.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Agriliance; AGSCP; BASF; Bayer CropScience; Dow AgroSciences; Helena; PBI Gordon; UAP-Platte; Micro Flo; Nufarm; Riverdale; Riverside/Terra; Wilbur-Ellis

Reference(s):

1. Ashton, F. M. and A. S. Crafts. 1981. Mode of Action of Herbicides, 2nd ed. Wiley-Interscience, New York.
2. Cole and Loughman. 1983. J. Exp. Bot. 34:1311.
3. Coupland, D. et al. 1990. Pestic. Biochem. Physiol. 36:61.
4. Kirkwood, R. C. et al. 1972. Pestic. Sci. 3:307.
5. Loussaert and Ellis. 1993. J. Plant Growth Regul. 12:47.
6. Lutman and Snow. 1987. Proc. Brit. Crop Prot. Conf.-Weeds, p. 901.
7. Peniuk, M. G. et al. 1992. Abstr. Weed Sci. Soc. Am. 32:55.
8. Slade, R. E. 1945. Nature (London) 155:498.
9. Tittle, F. L. et al. 1990. Plant Physiol. 94:1143.
10. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
11. Webb and Hall. 1993. Abstr. Weed Sci. Soc. Am. 33:66.

MCPB

4-(4-chloro-2-methylphenoxy)butanoic acid

CAS # Acid: 94-81-5
Sodium salt: 6062-26-6

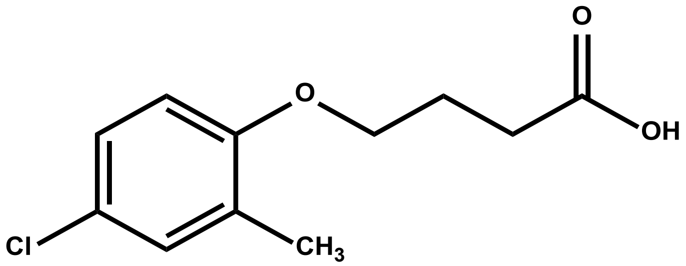
$4^{(O)}$

NOMENCLATURE

Common name: MCPB (BSI, ISO, WSSA)
Other name(s): MB 3046; 2,4-MCPB; 2M-4Kh-M; 4-(4-chloro-*o*-tolyloxy)butyric acid (IUPAC); 4-(2-methyl-4-chlorophenoxy)butyric acid
Trade name(s): CAN-TROL; LEGUMEX; PDQ; THISTROL®; TROPOTONE; TROPOTOX
Chemical family: phenoxy; phenoxyalkanoic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
MCPB acid



Molecular formula: *Acid* $C_{11}H_{13}ClO_3$; *Na salt* $C_{11}H_{12}ClNaO_3$
Molecular weight: *Acid* 228.68 g/mole; *Na salt* 250.66 g/mole
Description: White crystalline solid when pure
Density: NA
Melting point: 100-101 C (pure)
Boiling point: NA
Vapor pressure: 5.77×10^{-5} Pa (20 C); 9.83×10^{-5} Pa (25 C)
Stability: NA
Solubility:
Acid
water practically insoluble (20 C)
organic solvents (20 C):

acetone soluble	ether soluble
benzene slightly soluble	ethanol soluble

carbon tetrachloride slightly soluble
Sodium salt
water 200,000 mg/L (estimated) (25 C) (8)
pK_a: 4.8 (weak acid)

HERBICIDAL USE

MCPB can be applied POST at 0.56-1.7 kg ae/ha in field peas for control of Canada thistle and control or suppression of certain annual broadleaf weeds including lambsquarters, pigweed spp., smartweed spp., and morningglory spp.

USE PRECAUTIONS

Fire hazard: THISTROL is aqueous and non-flammable.
Corrosiveness: Non-corrosive
Storage stability: No limitations
Cleaning glassware/spray equipment: Flush with detergents, dilute alkali, and water
Incompatibilities: Possibly incompatible with hard water.

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood but similar to that of endogenous auxin (IAA) and other auxin-type herbicides (more details on page 12)
Symptomology: Symptoms include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 3-5 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.
Absorption: Foliar penetration of MCPB is slower than that of MCPA (apparently because of greater partitioning of MCPB into wax), and this may account for greater susceptibility of broad bean (*Vicia faba*) to MCPA (4). MCPB applied as a salt is protonated in the acidic environment outside the plasmalemma, and readily penetrates the plasmalemma as the protonated acid. Once inside the cell, the more-alkaline cytoplasm causes dissociation to produce MCPB anion which is trapped inside the cell due to its reduced ability to traverse the plasmalemma. Higher lipophilicity of MCPB and its more efficient penetration of mitochondrial membranes may account for its greater toxicity to lower vascular plants compared to MCPA (3).
Translocation: MCPB is transported primarily in the symplastic pathway (including the phloem), accumulating at the growing points. Translocation rate in tolerant species appears to be slower, perhaps because of the formation of immobile complexes, reduced xylem transport, and anatomical differences among species (1).
Metabolism in plants: MCPB is essentially non-toxic and must be activated by β-oxidation of the butyric acid side chain to form the phytotoxic MCPA in a reaction analogous to the conversion of 2,4-DB to 2,4-D. MCPB has greater species selectivity than MCPA because not all species convert MCPB to MCPA. Metabolism of MCPA derived from MCPB probably proceeds by hydroxylation of the 2-methyl group of MCPA to form (4-chloro-2-hydroxymethyl-phenoxy)acetic acid which then can be conjugated to glucose. Formation of the glucose ester of MCPA also has been reported, as well as conjugates with aspartic acid and perhaps other amino acids (1).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Mecoprop and MCPA resistance in a biotype of common chickweed has occurred in Britain (6). The mechanism of resistance appears to involve rapid herbicide metabolism and subsequent formation of non-herbicidal conjugates (2). This chickweed biotype likely is resistant to MCPB.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 20 mL/g (estimated) at pH 7 for the Na salt (8).

Transformation: NA

Persistence: Typical field half-life is 14 d (8)

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade MCPB acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 680 mg/kg; Dermal LD_{50}, NA; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

MCPB sodium salt: Oral LD_{50} rat, 690 mg/kg

Subchronic toxicity:

2-mo dietary, mouse: NOEL NA; lower body weight gains at 400 mg/kg/d

Chronic toxicity: NA

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Honey bee, non-toxic; Fathead minnow 96-h LC_{50}, 62 mg/L; Rainbow trout 96-h LC_{50}, 11 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React 2-methyl-4-chlorophenol with butyrolacetone in the presence of concentrated NaOH.

Purification of technical: Repeated crystallization from ethylene dichloride.

Analytical methods: Total chlorine by Parr Bomb as for 2,4-D or 2,4,5-T with suitable adaptations for MCPB molecular weight (Official Methods of Analysis AOAC, 11th Ed. 1970. Section 6.154-6.157, pp. 94-95.). Residue method can be found in PAM, Vol. II. Sec. 180.318.

Historical: First reported in 1955 (7). Introduced by May & Baker Ltd; British patent 758,980.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Nufarm

Reference(s):

1. Ashton, F. M. and A. S. Crafts. 1981. Mode of Action of Herbicides, 2nd Ed. Wiley-Interscience, New York.
2. Coupland, D. et al. 1990. Pestic. Biochem. Physiol. 36:61.
3. Kirkwood, R. C. et al. 1966. Pages 287-302 *in* Physico-Chemical and Biophysical Factors Affecting the Activity of Pesticides. Soc. Chem. Ind., Monogr. 29.
4. Kirkwood, R. C. et al. 1972. Pestic. Sci. 3:307.
5. Lutman and Snow. 1987. Proc. Brit. Crop Prot. Conf.-Weeds, p. 901.
6. Tittle, F. L. et al. 1990. Plant Physiol. 94:1143.
7. Wain and Wightman. 1955. Proc. Roy. Soc. 142B:525.
8. Wauchope, R. D. et al. 1992. Environ. Contam. Toxicol. 123:1.

mecoprop

2-(4-chloro-2-methylphenoxy)propanoic acid

CAS # Acid: 7085-19-0
P acid (*R* isomer): 16484-77-8

$4^{(O)}$

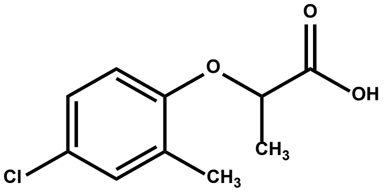
NOMENCLATURE

Common name: mecoprop (BSI, ISO, WSSA)
Other name(s): CMPP; MCPP; mechlorprop; RD 4593; *mecoprop* *dl*-2-(4-chloro-2-methylphenoxy)propionic acid; (*RS*)-2-(4-chloro-*o*-tolyloxy)propionic acid (IUPAC); 2-[(4-chloro-*o*-tolyl)oxy]propionic acid; 2-(2-methyl-4-chlorophenoxy)propionic acid; (±)-2-[(4-chloro-*o*-tolyl)oxy] propionic acid; *mecoprop-P* (2*R*)-2-(4-2-mehtylphenoxy) propanoic acid; (*R*)-2-(4-chloro-*o*-tolyloxy)propionic acid
Trade name(s): BELGRAN; CAMBILENE; COMPITOX; CORNOX PLUS; DISSOLVE®; ENDRUN; FOXPRO DT; FOXTRIL SUPER; ENCORE® DSC; KILPROP; ISO-CORNOX S7; MALERBANE; MCPP-4 AMINE; MCPP-80™ AMINE; MECOPEX; MEC AMINE-D®; MECAMINE PLUS™; MEPRO; METHOXONE M; MECOMEC®; SPRINGCLENE Z; SUPER TRIMEC®; OXYTRIL M; TRIMEC® SOUTHERN; TRIMEC® 992; TRIMEC® BENTGRASS FORMULA; TRIMEC® BRUSH KILLER; TRIMEC® CLASSIC; TRIMEC® ENCORE; TRIMEC® LAWN WEED KILLER; TRIMEC® PLUS; TRIMEC® TURF; TURF SUPREME + TRIMEC®; TRIAMINE®; TRIAMINE II; TRIESTER™; TRIESTER II; TRIPLET™; TRI-POWER®; TRI-POWER DRY; PROPONEX-PLUS; U-46 KY-FLUID; WINTACORN EXTRA
Chemical family: phenoxy; phenoxyalkanoic acid

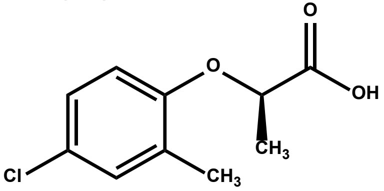
CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

mecoprop acid



Mecoprop-P



Molecular formula: *Acid* $C_{10}H_{11}ClO_3$; *Dimethylamine (Dma) salt* $C_{12}H_{18}ClNO_3$; *K salt* $C_{10}H_{10}ClKO_3$
Molecular weight: *Acid* 214.65 g/mole; *Dma salt* 259.73 g/mole; *K salt* 252.74 g/mole
Description: Colorless crystalline solid, odorless
Density: NA
Melting point: 94-95 C (pure); ≥ 90 C (technical)
Boiling point: NA
Vapor pressure: 3.1×10^{-4} Pa (20 C)
Stability: NA
Solubility:
Acid
water 620 mg/L (20 C)
Dimethylamine salt
water 660,000 mg/L (pH 7, 20 C)
pK_a: 3.11 (weak acid) (2)
K_{ow}: 1.26 (pH 7)

HERBICIDAL USE

Mecoprop can be applied POST at 2.24-3.36 kg ae/ha in established turf, and POST at 1.5-2.7 kg ae/ha in cereal crops. It controls several annual and perennial broadleaf weeds including chickweed spp., clover spp., plantain spp., knotweed spp., lambsquarters, pigweed spp., and ground ivy.

USE PRECAUTIONS

Fire hazard: Mecoprop technical and formulated products are dry or aqueous and non-flammable.
Corrosiveness: Mecoprop acid corrodes metal in the presence of water. Solutions of the K salt do not corrode brass, iron, and mild steel at pH >8.6. Slow corrosion may occur when temperatures approach 80 C.
Storage stability: Solutions of the K salt of mecoprop are stable for several years under normal storage conditions. At low temperatures, the K salt crystallizes, but the crystals re-dissolve on warming.
Cleaning glassware/spray equipment: Rinse with water containing a detergent.
Emergency exposure: Symptomatic treatment and removal of poison by gastric lavage. If ingested, induce vomiting.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood but similar to that of endogenous auxin (IAA) (more details on page 12)
Symptomology: Symptoms include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 3-5 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.
Absorption: Mecoprop can be washed off the leaf surface by rain occurring soon after application. Foliar penetration rate is relatively slow. Only 40% of applied mecoprop penetrated the leaf surface of common chickweed by 72 h after application (3). Mecoprop applied as a salt is protonated in the acidic environment outside the plasmalemma, and readily penetrates the plasmalemma as the protonated acid.

Once inside the cell, the more-alkaline cytoplasm causes dissociation to produce mecoprop anion which is trapped inside the cell due to its reduced ability to traverse the plasmalemma.

Translocation: Mecoprop is transported primarily via the symplastic pathway (including the phloem), accumulating at the growing points. Translocation rate appears to be slow as only 3, 10, and 4% of foliar-absorbed mecoprop was found in apical, basal, and root samples, respectively, of chickweed 72 h after treatment (3). Most of the absorbed mecoprop remained in the treated leaf.

Metabolism in plants: Mecoprop is metabolized fairly rapidly in chickweed (3). Between 63 and 94% of applied mecoprop was apparently converted to conjugated forms of the herbicide by 72 h after treatment. Over 99% of absorbed mecoprop was metabolized in barley by 3 wk after application, producing conjugates (attached at the carboxyl moiety) with amino acids, proteins, or sugars (1).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Mecoprop resistance in a biotype of common chickweed has occurred in Britain (7). The mechanism of resistance may involve increased metabolism and formation of nonherbicidal conjugates (3). Resistant chickweed biotypes produce higher ethylene levels than in susceptibles (4). Higher ethylene levels could enhance activity of malonyltransferase. Increased malonylation of mecoprop conjugates could stimulate sequestration in the vacuole.

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BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 20 mL/g (estimated) at pH 7 (9)

Transformation: NA

Persistence: Average field half-life is 21 d (9). Grasses can be planted 3-4 wk after application of mecoprop at recommended rates; however, only slight reduction in emergence occurs 1-2 wk after application.

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade mecoprop acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} mouse, 650 mg/kg; Dermal LD_{50} rabbit, 900 mg/kg; 4-h inhalation LC_{50} NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

Mecoprop Na salt technical: Oral LD_{50} mouse, 650 mg/kg; Dermal LD_{50} rabbit, 900 mg/kg

Subchronic toxicity: NA

Chronic toxicity:

7-mo dietary, rat: NOEL NA; slight enlargement of the kidneys at up to 100 mg/kg; slight anemia and kidney enlargement at 400 mg/kg

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife: NA

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Recrystallization**Analytical methods:** Analysis of mecoprop is by GLC of the methyl ester.

Historical: Plant growth regulating activity was described in 1953 (5) and its use as a herbicide in 1956 (6). Introduced by The Boots Co. Ltd; British patents 820,180, 822,973, and 825,875.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience; Helena; PBI Gordon; Riverdale; J. R. Simplot; UAP-Platte

Reference(s):

1. Cessna, A. J. 1992. J. Agric. Food Chem. 40:1154.
2. Cessna and Grover. 1978. J. Agric. Food Chem. 26:189.3. Coupland, D. et al. 1990. Pestic. Biochem. Physiol. 36:61.
4. Coupland and Arnold. 1992. Pestic. Sci. 34:365.
5. Fawcett, C. H. et al. 1953. Ann. Appl. Biol. 40:232.
6. Lush and Leafe. 1956. Proc. 3rd Br. Weed Control Conf. pp. 625, 633.
7. Lutman and Snow. 1987. Proc. Brit. Crop Prot. Conf.-Weeds, p. 901.
8. Tittle, F. L. et al. 1990. Plant Physiol. 94:1143.
9. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

mefenacet

CAS #: 73250-68-7

$15^{(K_3)}$

2(2-benzothiazolyloxy)-*N*-methyl-*N*-phenylacetamide

NOMENCLATURE

Common name: mefanacet

Other name(s): bensaicaoan; BAY FOE 1976; 2-(1,3-benzothiazol-2-yloxy)-*N*-methylacetanilide (IUPAC); 2-benzothiazol-2-yloxy-*N*-methylacetanilide (IUPAC)

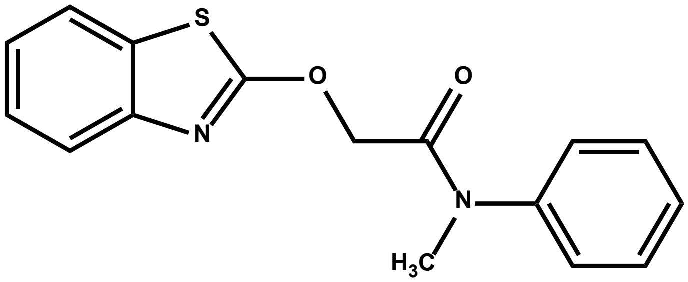
Trade name(s): ACT; HINOCHLOA; MANSOKUM; LEEDZON; RANCHO; SIUZAN; ZARK

Chemical family: acetamide; anilide; oxyacetamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

mefenacet



Molecular formula: $C_{16}H_{14}N_2O_2S$

Molecular weight: 298.36 g/mole

Description: Colorless, odorless crystals

Density: NA

Melting point: 134.8 C

Boiling point: NA

Vapor pressure: 6.4×10^{-7} Pa (20 C)

Stability: Stable to light. Less than 5% degraded after 6 mo (30 C)

Solubility:

water, 4 mg/L (20 C)
dichloromethane >200 mg/L
hexane 0.1-1.0 mg/L
toluene 20-50 mg/L.

pK_a: None (non-ionizable)

K_{ow}: 1700

HERBICIDAL USE

Mefenacet is used for control of grass weeds, especially *Echinochloa crus-galli* and broadleaf weeds in transplanted rice. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: NA

Storage stability: NA

Emergency exposure: NA

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of shoot growth; recently has been shown to inhibit very long chain fatty acid synthesis (more details on page 14)

Symptomology: Inhibition of seedling growth

Absorption/translocation: Absorbed by roots; primarily xylem translocated

Metabolism in plants: Metabolized to 4-aminophenol via oxidation of an intermediate *N*-methylaniline.

Mechanism of resistance in weeds: No resistance reported

BEHAVIOR IN SOIL

Sorption:

K_d: Ranged from 29 to 420 mL/g (1)

Transformation:

Other degradation: Menfenacet undergoes slow hydrolysis at all pH levels.

Persistence:

Field experiments: DT_{50} few weeks

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade mefenacet unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50} rats, >0.02 mg/L; non-irritating to skin or eyes

Chronic toxicity:

24-mo dietary, mouse: NOEL 300 mg/kg diet; rats: NOEL 100 mg/kg diet.

Wildlife:

Bobwhite quail LC_{50} (5 d), >5000 mg/kg diet; carp LC_{50} (96 h), 6.0 mg/L; trout 6.8 mg/L; golden orfe, 11.5 mg/L; worms LC_{50} (28 d), >1000 mg/kg/d dry substrate; Daphnia LC_{50} (48 h), 1.81 mg/L

Use classification: WHO class III; EPA (formulation) IV.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Kibe, K. et al. 2000. Sci. Total Environ. 263:115-125

mefenpyr-diethyl

CAS #: 135590-91-9 **NC**

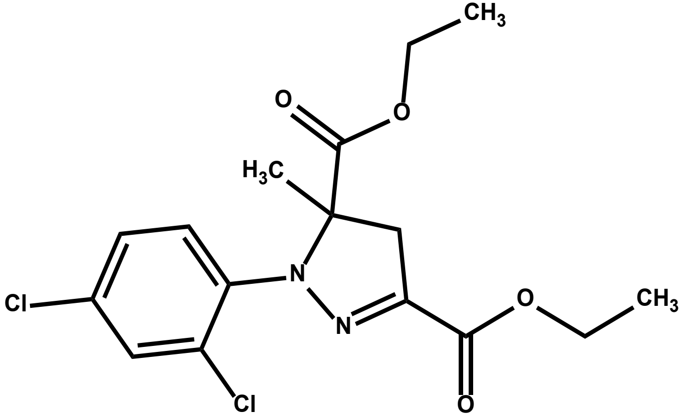
diethyl 1-(2,4-dichlorophenyl)-4,5-dihydro-5-methyl-1*H*-pyrazole-3,5-dicarboxylate

NOMENCLATURE

Common name: mefenpyr-diethyl (ISO)
Other name(s): AEF 107892; diethyl (*RS*)-1-(2,4-dichlorophenyl)-5-methyl-2-pyrazoline-3,5-dicarboxylate
Trade name(s): NA
Chemical family: NA

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
mefenpyr-diethyl



Molecular formula: $C_{16}H_{18}Cl_2N_2O_4$
Molecular weight: 373.24 g/mole
Description: white to light beige crystals
Density: 1.31 g/mL (20 C)
Melting point: 50 – 52 C
Boiling point: NA
Vapor pressure: 6.3 Pa (20 C)
Stability: Hydrolyzed by acids and alkali
Solubility: In water, 20 mg/kg pH 6.2 (20 C). In acetone > 500 g/L, toluene > 400 g/L, ethyl acetate > 400 g/L, methanol > 400 g/L
pK_a: None (non-ionized)
K_{ow}: log K_{ow} = 3.83 (pH 6.3, 21 C)

HERBICIDAL USE

Mefenapyr-diethyl is used as a safener in combination with fenoxaprop-P-ethyl and iodosulfuron (1:3 mixture of iodosulfuron to mefenpyr-diethyl) for selective weed control in wheat, rye, triticale, and some barley varieties.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: NA
Symptomology: NA
Absorption/translocation: NA
Metabolism in plants: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Transformation:
Photodegradation: DT_{50} 2.9 d at 52° N latitude
Other degradation: Hydrolysis contributes to mefenpyr-diethyl degradation in soil.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >4000 mg/kg; non-irritating to skin and eyes
Mutagenicity: non-mutagenic
Wildlife:
Acute oral LD_{50} for Japanese quail, >2000 mg/kg; carp LC_{50} (96 h), 2.4 mg/L; rainbow trout, 4.2 mg/L; bees LD_{50} (oral, 48 h), >900 µg/bee; Worms LC_{50} (14 d), >1000 mg/kg soil; Daphnia LC_{50} (48 h), 53 mg/l
Use classification: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1. Hacker, E., H. Bieringer, L. Willms, O. Ort, H. Koecher, H. Kehne, and R. C. Fisher. 1999. Proc. Br. Corp Prot. Conf. – Weeds Vol. 1:15-22.

mefluidide

N-[2,4-dimethyl-5-[[(trifluoromethyl)sulfonyl]amino]phenyl] acetamide

CAS # Acid: 53780-34-0
Diethanol amine salt: 53780-36-2

NC

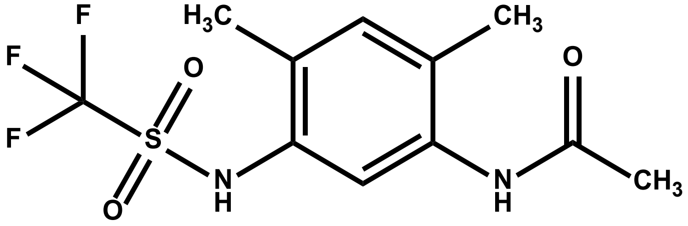
NOMENCLATURE

Common name: mefluidide (BSI, ISO, WSSA; ANSI as a plant growth regulator)
Other name(s): MBR 12325; 5′-(1,1,1-trifluoromethanesulfonamido)acet-2′,4′-xylidide (IUPAC)
Trade name(s): EMBARK®; EMBARK LITE; VISTAR®
Chemical family: anilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

mefluidide acid



Molecular formula: *Acid:* $C_{11}H_{13}F_3N_2O_3S$; *Diethanolamine (Dea) salt:* $C_{15}H_{24}F_3N_3O_5S$
Molecular weight: *Acid:* 310.29 g/mole; *Dea salt:* 415.43 g/mole
Description: White solid, odorless
Density: *Dea salt:* 0.69 g/mL (25 C)
Melting point: *Acid:* 183-185 C; *Dea salt:* 106-108 C
Boiling point: NA
Vapor pressure: *Dea salt:* $<1.3 \times 10^{-5}$ Pa (25C)
Stability: *Dea salt:* Stable (25-150 C) in air or N_2
Solubility:

water 180 mg/L (23 C)
organic solvents g/100 mL (23 C):
acetone 35
acetonitrile 6.4
benzene 0.031
DMSO 68
diethyl ether 0.39
ethyl acetate 5
methanol 31
methylene chloride 0.21
petroleum benzene 0.0002

pK_a: 4.6 (25.6 C)
K_{ow}: *Dea salt* 0.032

HERBICIDAL USE

Mefluidide is applied POST at 0.14-1.12 kg ae/ha as a plant growth regulator to suppress seedhead formation and vegetative growth of cool and warm season turfgrasses. It also can be applied POST with spray-to-wet treatments at 0.125-0.5% v/v to inhibit vegetative growth and fruit set of ornamental shrubs, hedges, trees, and groundcovers. These applications generally reduce mowing or trimming requirements by 6-8 wk. Herbicidal uses of mefluidide have been discontinued.

USE PRECAUTIONS

Fire hazard: All formulated products are aqueous and nonflammable.
Corrosiveness: EMBARK 2-S is slightly corrosive to metallic sprayer parts upon prolonged contact.
Storage stability: EMBARK 2-S and EMBARK LITE were stable at 60 C for up to 9 mo. Formulations should be stored at >4 C.
Cleaning glassware/spray equipment: Rinse with household ammonia and water.
Emergency exposure: If ingested, induce vomiting.
Incompatibilities: Will precipitate if mixed with liquid fertilizers or with pesticides that are weak acids (pK_a <5).

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Growth and development of meristems of responsive plants are inhibited. Mefluidide may inhibit conversion of geranylgeraniol to *ent*-kaurenol, thereby blocking gibberellic acid (GA) biosynthesis (6), although GA application does not reverse growth inhibition by mefluidide (5). Increases in polar transport of IAA (4) and changes in the lipid composition of cell membranes suggest that mefluidide may interfere with membrane function.
Symptomology: Foliar growth inhibition. Crown and leaf bases of grasses may thicken and twist. Low concentrations may stimulate growth and tillering in grasses.
Absorption/translocation: Absorbed readily into leaves but less so into roots. Leaf absorption is increased greatly by surfactants or high humidity. Substantial percentages of leaf-absorbed mefluidide are translocated (apparently in the phloem) to growing points in the shoot but less so to roots. Root-absorbed mefluidide translocates acropetally (apparently in the xylem), but at low to moderate percentages of absorbed. It accumulates primarily in older leaves (2, 3).
Metabolism in plants: Mefluidide had a half-life in tall fescue of about 7 d. However, no metabolites were detected 3,7, and 14 d after treatment, indicating that metabolites were rapidly degraded or were incorporated into non-extractable residues. Mefluidide was metabolized 14% in corn coleoptiles and 54% in soybean hypocotyls after 6 h, apparently to a conjugate releasing parent mefluidide upon acid treatment (4).
Non-herbicidal biological properties: Mefluidide primarily is used as a growth regulator, with some herbicidal effects at higher rates; may synergize the activity of certain herbicides
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Not strongly adsorbed to soil; adsorption to OM is greater than to clay, and adsorption is greater at lower soil pH.

K_{oc}: Average is 200 mL/g (estimated) (1)

Transformation:

Photodegradation: Not appreciably degraded on dry soil surfaces, but photodegrades significantly when dissolved in water.

Persistence: Rapidly degraded in soil, with a half-life of 2 d.

Mobility: Mefluidide is leachable; OM and soil acidity retard leaching.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade mefluidide acid unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >4000 mg/kg; mouse, 1920 mg/kg; Dermal LD_{50} rabbit, >4000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Mefluidide diethanolamine salt: 4-h inhalation LC_{50} rat, >8.5 mg/L

Subchronic toxicity:

90-d dietary, rat: NOEL 6000 mg/kg

90-d dietary, dog: NOEL 1000 mg/kg

Chronic toxicity:

18-mo dietary, mouse: NOEL 600 mg/kg

24-mo dietary, rat: NOEL 600 mg/kg

Teratogenicity:

Rat: NOEL 1800 mg/kg**Rabbit:** NOEL NA; not teratogenic at 15, 30, and 60 mg/kg/d

Reproduction:

Rat: NOEL 1800 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative

DNA damage/repair: Two unspecified tests, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck oral LD_{50}, >4640 mg/kg; 8-d dietary LC_{50}, 10,000 mg/kg; Honey bee oral LD_{50}, >75 µg/bee; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Following extraction, mefluidide is derivatized with diazomethane and analyzed by GC with flame ionization detection.

Historical: Mefluidide was discovered at 3M Company while researching the *N*-aryl 1,1,1-trifluoro-methanesulfon amides; U.S. patent 3,894,078.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): PBI Gordon

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Bloomberg and Wax. 1978. Weed Sci. 26:434.
3. McWhorter and Wills. 1978. Weed Sci. 26:382.
4. Glenn and Rieck. 1985. Weed Sci. 33:452.
5. Truelove, B. et al. 1977. Weed Sci. 25:360.
6. Wilkinson, R. E. 1982. J. Plant Growth Regul. 1:85.

mesosulfuron

CAS #:: 208465-21-8 **$2^{(B)}$**

Methyl 2-[[[[(4,6-dimethoxy-2-pyrimidinyl) amino]carbonyl] amino]sulfonyl]-4-[[(methylsulfonyl)amino]methyl]benzoate

NOMENCLATURE

Common name: mesosulfuron-methyl

Other name(s): methyl 2-[(4,6-dimethoxypyrimidin-2-ylcarbamoyl)sulfamoyl]-amesosulfuron (methanesulfonamido)-p-toluate (IUPAC)

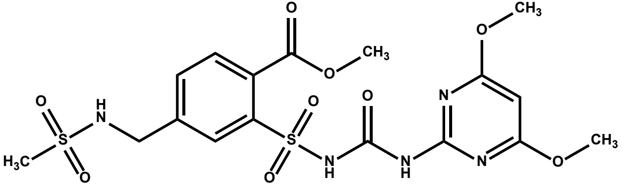
Trade name(s): MESOMAXX, ATLANTIS, OSPREY, SILVERADO

Chemical family: sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

Mesosulfuron-methyl



Molecular formula: $C_{17}H_{21}N_5O_9S_2$

Molecular weight: 503.51 g/mole

Description: cream color powder

Density: 1.53 g/ml at 23 °C

Melting point: 189-192 °C

Boiling point: decomposes before boiling

Vapor pressure: 1.1×10^{-11} Pa (25 C)

Stability: No significant change in the AI content (2.2% decrease) when stored for 14 days at 540C.

Solubility:

Water: 483 at 20 °C

Organic solvents mg L^{-1} (20°C)

Hexane	200
Acetone	13660
Ethyl acetate	2000
Toluene	130

pK_a: 4.35 at 20 °C

K_{ow}: log K_{ow} = 1.9 at pH 4

HERBICIDAL USE

Mesosulfuron is registered for selective postemergence grass and broadleaf weed control in wheat

USE PRECAUTIONS

Fire hazard: Nonflammable

Corrosiveness: NA

Storage stability: NA

Cleaning glassware/spray equipment: NA

Emergency exposure: .NA

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: ALS inhibitor (see other ALS inhibitors) (more details on page 12)

Symptomology: NA

Absorption/translocation: NA

Metabolism in plants: NA

Non-herbicidal biological properties: NA

Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA

Transformation: NA

Photodegradation: NA

Other degradation: .NA

Persistence: pH and temperature sensitive: DT50 7.2 days at pH 5 and 20 degC, 3.5 days at pH 5 and 25 degC, 253 days at pH 7 and 25 deg C, 23 days at pH 7 and 40 degC, 318 days at pH 9 and 25 deg C, 27 dats at pH 9 and 40 degC

Field experiments:

Mobility: high leachability

Volatilization: non-volatile

TOXICOLOGICAL PROPERTIES

.Acute toxicity:

Oral

Mammals >5,000 mg/kg

Dermal

Mammals >5,000 mg/kg

Inhalation

Mammals >1.33 mg l^{-1}

Subchronic toxicity:

Chronic toxicity:

Teratogenicity:

Reproduction:

Mutagenicity:

Wildlife:

freshwater fish LC_{50} > 91.5 ppm

freshwater aquatic invertebrates LC_{50} > 90.2 ppm

bobwhite quail and mallard duck LD_{50} > 2,000 mg/kg

honey bee LD_{50} > 13 ug/bee

Use classification:

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

mesotrione

CAS #: 104206-82-8

$27^{(F_2)}$

2-[4-(methysulfonyl)-2-nitrobenzoyl]-1,3-cyclohexanedione

NOMENCLATURE

Common name: mesotrione

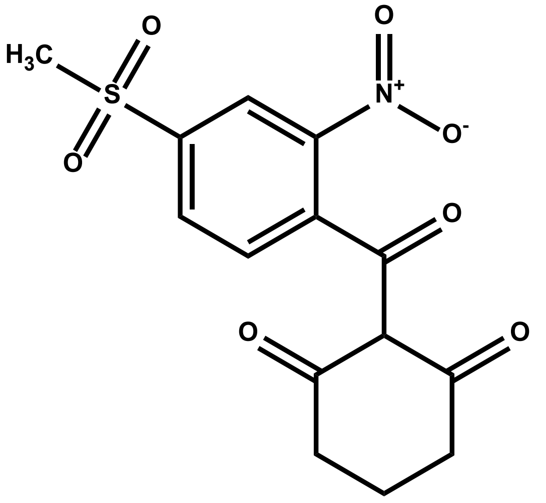
Other name(s): 2-(4-mesyl-2-nitrobenzoyl)cyclohexane-1,3-dione (IUPAC)

Trade name(s): CALLISTO®. LUMAX®; CAMIX®; CALARIS®; LEXAR®; HALEX GT®; ELUMIS®

Chemical family: benzoylcyclohexanedione; triketone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *mesotrione*



Molecular formula: $C_{14}H_{13}NO_7S$

Molecular weight: 339.32 g/mole

Description: Light tan solid

Density: 1.46 g/mL (20 C)

Melting point: 165 C; slowly decomposes on melting

Boiling point: NA

Vapor pressure: 5.69×10^{-6} Pa

Stability: Stable to hydrolysis (pH 4-9)

Solubility:

water 2200 mg/L (pH 4.8, 20 C); 15,000 mg/L (pH 6.9, 20 C); 22,000 mg/L (pH 9, 20 C)

pK_a: 3.12 (weak acid)

K_{ow}: NA

HERBICIDAL USE

Premergence (100-225 g/ha) and postemergence (70-150 g/ha) control of broadleaf weeds like *Xanthium*, *Abutilon*, *Chenopodium*, *Polygonum*, and *Ambrosia trifida* and some grass weeds in maize. Some utility in rice one-shot products in Asia.

USE PRECAUTIONS

Fire hazard: May degrade, decompose exothermically and even catch fire when exposed to temperatures in excess of 60 C. Flammable dust clouds may form.

Corrosiveness: Non-oxidizing

Storage stability: Keep away from heat and direct sunlight. Product may decompose

Emergency exposure: On ingestion, do not induce vomiting, seek medical attention. On eye contact, irrigate eyes for at least 15 min with water/eyewash solution.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme 4-hydroxyphenyl-pyruvate dioxygenase (4-HPPD) affecting carotenoid biosynthesis (more details on page 15)

Symptomology: Symptoms in sensitive plants include bleaching followed by necrosis within 3-5 d.

Absorption/translocation: Absorbed through the shoot and can be absorbed through the root following post-emergence applications. It is absorbed via the seed and emerging root and shoot following pre-emergence applications. It is translocated in xylem and phloem and distributed throughout the plant in weed species.

Metabolism in plants: Corn rapidly metabolizes mesotrione to inactive metabolites. Cytochrome P450 enzymes mediate mesotrione detoxification in plants. Major metabolites are conjugates of MNBA and AMBA. Lower rates of foliar uptake in corn as compared to weeds could also contribute to selectivity.

Non-herbicidal biological properties: NA**Mechanism of resistance in weeds:** Very low risk for site of action resistance to mesotrione, the typical type of resistance observed with ALS and triazine herbicides.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 14-390 mL/g

Transformation:

Photodegradation: Aqueous photolysis half-life of 84 days. Soil photolysis half-life of 15-21 d.

Other degradation: Mesotrione is rapidly degraded in soil by microorganisms primarily to CO_2. In anaerobic conditions and in water, Mesotrione is also rapidly degraded by microorganisms. The mean soil half-life ranges from 5 to 15 days for mesotrione and is less than 6 days for each metabolite (MNBA and AMBA). Average field soil half-life (DT_{50}) is approx. 9 d.

Mobility: The potential; for mesotrione to leach is negligible. Mobility may occur on soils of high pH, due to low adsorption. In practice, these conditions lead to greater microbial availability and more rapid degradation. No mobility has been observed under field conditions-rapid degradation and low use rate mean there is little potential of ground water contamination and run-off is small.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade mesotrione unless otherwise indicated.

Acute toxicity:

Rats LD_{50}, >5000 mg/kg; Dermal LD_{50} rats, >2000 mg/kg; (4-h) inhalation LC_{50} rats, >5 mg/L; Eye irritation rabbit, mild; Skin irritation rabbit, practically none; Skin sensitization guinea pig, no.

Teratogenicity: Not teratogenic

Reproduction: No adverse reproductive effects

Mutagenicity: Not mutagenic/carcinogenic

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purfication of technical: NA

Analytical methods: NA

Historical: Introduced by Syngenta in the US in 2001.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry souce(s): Syngenta Crop Protection

metaborate

sodium metaborate dodecahydrate

CAS #: 7775-19-1

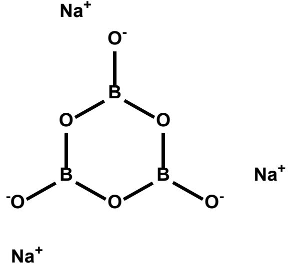
NC

NOMENCLATURE

Common name: metaborate
Other name(s): borate; sodium metaborate
Trade name(s): BAREGROUND BD; BARESPOT® WEED & GRASS; BARESPOT MONOBOR-CHLORATE; BARESPOT UREABOR; BOROCIL IV PRAMITOL® 5PS; PROMETON 5PS; TOTAL™
Chemical family: none generally recognized

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
sodium metaborate (non-hydrated)



Molecular formula: $B_3Na_3O_6\cdot 12H_2O$ (hydrated)
Molecular weight: 128.43 g/mole (non-hydrated)
Description: White solid, odorless
Density: 1.90 g/mL (25 C)
Melting point: Water of hydration melts at 57 C; dehydrated metaborate melts at 966 C
Boiling point: 1400 C
Vapor pressure: NA
Stability: Stable to UV light
Solubility:
water 260,000 mg/L (20 C)
pK_a: NA
K_{ow}: NA

HERBICIDAL USE

Borate can be applied before or after weed emergence at 85-224 kg ai/ha in mixture with other herbicides for total vegetation control on non-crop land such as industrial sites, rights-of-way, fence lines, lumberyards, etc.

USE PRECAUTIONS

Fire hazard: All products are dry and nonflammable
Corrosiveness: Solutions do not corrode ferrous metals
Storage stability: Stable
Cleaning glassware/spray equipment: Water or steam
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Unknown. Similarity between symptoms caused by metaborate injury and calcium deficiency have led to speculation that metaborate may bind plant calcium(1).
Symptomology: Necrosis begins in the leaf margins followed by desiccation throughout the leaf. Young plants are most sensitive (1).
Absorption/translocation: Readily absorbed by leaves, but poorly translocated to other plant parts. Metaborate also can be absorbed by roots and translocated through the xylem to all foliar organs with accumulation in the leaves.
Metabolism in plants: NA
Non-herbicidal biological properties: Insecticidal, fungicidal, and nematocidal activity at high concentrations.
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Some adsorption of borate on clay
Transformation:
Photodegradation: No losses
Other degradation: Elemental boron cannot be degraded.
Persistence: Highly persistent since elemental boron cannot be degraded.
Mobility: Rapid leaching in high rainfall areas.
Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade sodium metaborate unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 2330 mg/kg; Dermal LD_{50}, NA; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, moderate; Skin sensitization, NA; Eye irritation, NA
Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife: NA
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Action of caustic soda on borax
Purification of technical: NA
Analytical methods: See (2)
Historical: Herbicidal activity of boron compounds was first reported in 1876 (3), but their use as herbicides began in the late 1930s (4).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; Agriliance; Helena; UAP-Platte; Pro-Serve; Riverside/Terra; J. R. Simplot; Syngenta Crop Protection

metamifop

CAS #: 256412-89-2 **$1^{(A)}$**

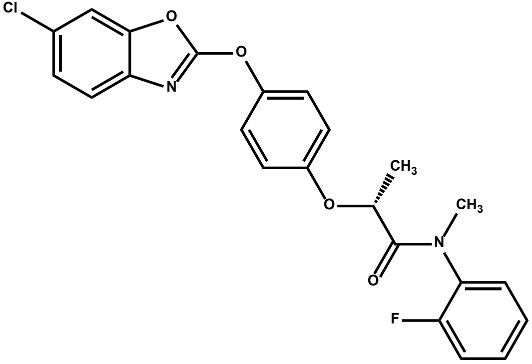
*(*2R)-2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]-N-(2-fluorophenyl)-N-methylpropanamide

NOMENCLATURE

Common name: metamifop \
Other name(s): DBH-129; K-12974; (R)-2-[4-(6-chloro-1,3-benzoxazol-2-yloxy)phenoxy]-2'-fluoro-N-methylpropionanilide (IUPAC)
Trade name(s): NA
Chemical family: anilide; aryloxyphenoxy propionate; aryloxyphenoxy propionic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
metamifop



Molecular formula: $C_{23}H_{18}ClFN_2O_4$
Molecular weight: 440.86 g/mole
Description: Pale brown powder
Density: NA
Melting point: 77.0-78.5 C
Boiling point: NA
Vapor pressure: 1.51×10^{-4} Pa (25 C); Henry's Law constant, 6.35×10^{-2} Pa m^3/mol (20 C)
Stability: NA
Solubility: 0.69 mg/L (pH 7, 20 C) in water
pK_a: NA
K_{ow}: log K_{ow} = 5.45 (pH 7, 20 C)

HERBICIDAL USE

Metamifop is applied postemergence in paddy and direct-seeded rice cultivation at rates of 90-200 g ai/ha to provide control of major grass weeds including *Echinochloa spp., Leptochloa chinensis, Digitaria spp.,* and *Eleusine indica* with excellent rice safety.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: Non-corrosive
Storage stability: NA
Cleaning glassware/spray equipment: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of Acetyl CoA carboxylase (ACCase) (more details on page 12)
Symptomology: In susceptible plants, chlorosis in developing leaves is accompanied by growth inhibition within a few days of application. Dependent upon the species, final death with severe desiccation occurs approximately 2 wks. after application.
Absorption/translocation: Foliar absorption of metamifp through the leaf surface of rice and barnyardgrass was almost complete within 24 h of application. Rice showed a lower foliar uptake of ^{14}C-metamifop than barnyardgrass 72 h after application. Translocation seems to move mainly through the xylem rather than through the phloem.
Metabolism in plants: The I_{50} values for ACCase inhibition by metamifop was >10 μM in rice and 0.5 ∝M in barnyardgrass. More ^{14}C-metamifop was absorbed through the leaf surface in barnyardgrass than in rice, with about 83% and 56% of the total applied metamifop penetrating 72 h after application, respectively. Differential selectivity of metamifop between rice and barnyardgrass could be due to both differential foliar absorption rate and differential ACCase sensitivity.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: The mechanism of resistance is an altered herbicide binding site in the ACCase target enzyme.

BEHAVIOR IN SOIL

Sorption: NA
K_{oc}: NA
Transformation:
Photodegradation: An aqueous photolysis study showed seven detectable metabolites identified by LC-MS and DT_{50} values ranging from 18 to 120 d in various water conditions.
Other degradation: In aerobic soil conditions, the half-life of metamifop is 40 to 60 d at 25 C. In anaerobic soil conditions, two major metablites of metamifop were found, HPFMPA and MFA metabolites. The HPFMPA metabolite was the major one found.
Persistence: In laboratory studies, the half-life of ^{14}C-metamifop in non-sterile and sterile soil was 53 and 78 d, respectively.
Mobility: NA
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical-grade metamifop unless otherwise indicated.
Acute toxicity:
LD_{50} >2000 mg/kg for rats; Dermal toxicity LD_{50} >2000 mg/kg for rats; Inhalation LC_{50} 2.61 mg/L for rats; non-irritant for skin and eye; not oncogenic or teratogenic in rats and mice.

Subchronic toxicity:
90-d dietary, rat: NA
21-d dermal, rabbit: NA
Chronic toxicity:
24-mo dietary, rat: NA
18-mo dietary, mouse: NA
12-mo dietary, dog: NA
Teratogenicity: NOEL (13 wks) 200 mg/kg for rats. Not oncogenic or teratogenic in rats or mice.
Rat: NA
Rabbit: NA
Reproduction:
Rat: NA
Mutagenicity:
Gene mutation: NA
Structural chromosome aberration: NA
Mammalian cell transformation: NA
Wildlife:
Daphnia magna LC_{50} (48 h) 0.288 mg/L; Honeybee LD_{50} >100 μg ai/bee (contact, dietary)
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA

Historical: Discovered by Korean Research Institute of Chemical Technology. Not sold in the United States and Canada.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dongbu Hannong Chemical Co.
Reference(s):

1. Kim, T. J., H. S. Chang, J. W. Ryu, Y. K. Ko, D. W. Kim, K. Y. Cho, C. H. Park, O. Y. Kwon, and B. J. Chung. 2003. Metamifop: A new post-emergence grass killing herbicide for use in rice. Proceedings BCPC – Crop Science & Technology. 1:81-86.
2. Kim, T. J., H. S. Chang, J. S. Kim, I. T. Hwang, K. S. Hong, D. W. Kim, K. Y. Cho, E. J. Myung, and B. J. Chung. 2003. Metamifop: mechanism of herbicidal activity and selectivity in rice and barnyardgrass. Proceedings BCPC – Crop Science & Technology. 2:833-838.
3. Chang, H. R., K. W. Yang, B. J. Chung, K. Kim, and Y. H. Kim. 2005. Anaerobic soil metabolism of ^{14}C-metamifop under chemical reducing conditions with sodium sulfide. Proceedings SETAC Conference. Abstract CHA-1117-597088.

metamitron

CAS #: 41394-05-2 $5^{(C_1)}$

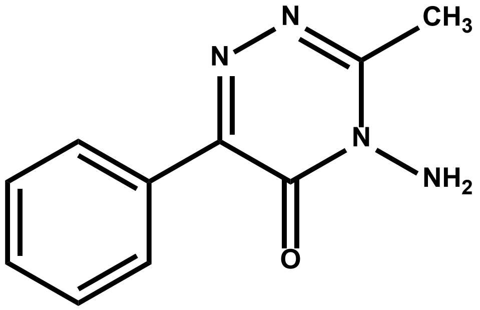
4-amino-3-methyl-6-phenyl-1,2,4-triazin-5(4H)-one

NOMENCLATURE

Common name: metamitron
Other name(s): metamitrone; 4-amino-3-methyl-6-phenyl-1,2,4-triazin-5(4H)-one (IUPAC); 4-amino-4,5-dihydro-3-methyl-6-phenyl-1,2,4-triazin-5-one (IUPAC)
Trade name(s): AQUILON®; DANAGAN; GOLTIX®; MARQUIS; MM-70; SKATER®; TORERO®; TORNADO®
Chemical family: triazinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
metamitron



Molecular formula: $C_{10}H_{10}N_4O$
Molecular weight: 202.2 g/mole
Description: Yellowish odorless crystals
Density: 1.35 g/mL (22.5 C)
Melting point: 166.9 g/mole
Boiling point: NA
Vapor pressure: 8.6×10^{-7} Pa (20 C)
Stability: Stable under normal temperatures and pressures
Solubility: water 1.7 g/L (20 C)
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 0.71

HERBICIDAL USE

Metamitron is used for PRE and POST control of grasses and broadleaf weeds in sugar and red beets, fodder beet, mangold and certain strawberry varieties. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: NA
Storage stability: NA
Cleaning glassware/spray equipment: NA
Emergency exposure: Skin contact: wash off immediately with soap and plenty of water; Eyes: rinse immediately with plenty of water; Ingestion: remove by inducing vomiting
Incompatibilities: Alkaline materials can cause hydrolysis; strong oxidizers can cause fire and explosion hazards.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Similar to other triazinone herbicides; leaves turn chlorotic, then necrotic after exposure
Absorption/translocation: Absorbed mainly by roots, but to some extent by leaves
Metabolism in plants: In sugar beet, deaminated metamitron is the major metabolite (1)
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Similar to that of other triazinone herbicides

BEHAVIOR IN SOIL

Sorption: K_{oc}: 91-392 mL/g
Transformation: Degradation in water-sediment systems is rapid. Most of the applied metamitron is degraded over 4-6 weeks.
Persistence: 4-6 weeks dissipation under normal conditions.
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, 2463 mg/kg; Dermal LD_{50} rats, >2000 mg/kg; Skin sensitization, none; Eye irritation, mild
Teratogenicity: Non-teratogenic
Mutagenicity: Non-mutagenic
Wildlife:
LC_{50} (96 h) rainbow trout, >143 mg/L; Acute LD_{50} oral bobwhite quail, >2000 mg/kg; Daphnia magna EC_{50} (48 h), > 50 mg/L; non-toxic to bees
Use classification: WHO (a.i.) III; EPA (formulation)

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA**Analytical methods:** HPLC
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience; Feinchemie Schwebda; United Phosphorus
Reference(s):

1. Roberts, T. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry. Bayer CropScience;

metazachlor

CAS #: 67129-08-2

15$^{(K_3)}$

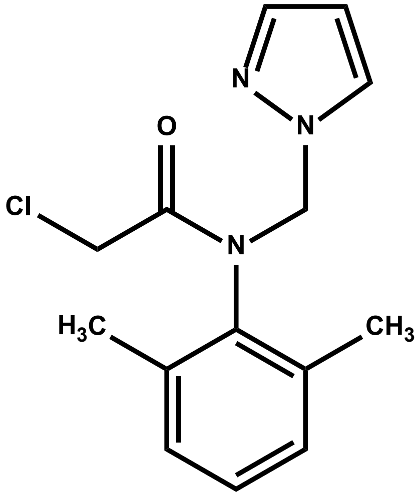
2-chloro-*N*-(2,6-dimethyphenyl)-*N*-(1*H*-pyrazol-1-ylmethyl) acetamide

NOMENCLATURE

Common name: metazachlor (BSI, ISO)
Other name(s): métazachlore (F-ISO); BAS 2903; BAS 479 00H; 2-chloro-*N*-(pyrazol-1-ylmethyl)acet-2',6'-xylidide (IUPAC)
Trade name(s): BUTISAN®; PUEGO®
Chemical family: acetamide; acetanilide; chloroacetamide; chloroacetanilide; pyrazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
metazachlor



Molecular formula: $C_{14}H_{16}ClN_3O$
Molecular weight: 277.75 g/mole
Description: Yellowish crystals
Density: 1.31 g/mL (C)
Melting point: 85 C
Boiling point: Not applicable
Vapor pressure: 9.3 x 10^{-5} Pa (20 C)
Stability: Stable for at least 2 yr at up to (40 C)
Solubility:
water 450 mg/L (20 C)
acetone >1000 g/kg
chloroform >1000
ethyl acetate 590
ethanol 200
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 2.49

HERBICIDAL USE

Metazachlor provides preemergence and early postemergence control of annual grasses and broadleaf weeds in transplanted brassicas, oilseed rape, potatoes, soybeans, ground-nut, maize, strawberries, sugarcane, cotton, and tobacco. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Non-corrosive**Storage stability:** NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Growth inhibition. Böger et al. (1) reports that metazachlor inhibits very long-chain fatty acid synthesis. (more details on page 14)
Symptomology: Inhibition of growth o f seedling plants.
Absorption/translocation: Absorbed by roots of germinating seedlings; translocated primarily by the xylem
Metabolism in plants: Metazachlor is metabolized by way of glutathione conjugation in tolerant plant species.
Mechanism of resistance in weeds: No reported resistance.

BEHAVIOR IN SOIL

Sorption:

$K_{oc:}$ 70-80 mL/g
Transformation:
Other degradation: At pH 5, 7, 9 at 22 C, hydrolytic DT_{50} is 766, 570, and 487 d in aqueous solution.
Persistence:
Field experiments: DT_{50} 1-3 mo
Lab experiments: DT_{50} 1-23 d

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade metazachlor unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 2150 mg/kg; Dermal LD_{50} rat, 6810 mg/kg; Acute 4-h inhalation LC_{50}, >4.5 mg/L; non-irritating to skin or eyes
Subchronic toxicity:
90-d dietary rat: NOEL 100 mg/kg bw
Chronic toxicity:
18-mo dietary, rat: NOEL 3.5 mg/kg bw
6-mo oral capsule, dog: NOEL 8 mg/kg bw
Teratogenicity:
Rat: maternal toxicity 150 mg/kg bw; developmental toxicity 450 mg/kg bw
Rabbit: Maternal 250 mg/kg bw
Mutagenicity: Negative
Wildlife:
Acute LD_{50} quail, >2000 mg/kg; LC_{50} (8 d), >5620 mg/kg bw; rainbow trout LC_{50} (96 h), 4 mg/L; honeybee LD_{50}, >1000 μg/bee; earthworm LC_{50}, 440 mg/kg soil
Use classification: WHO class 5 – unlikely to be hazardous under normal use

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): BASF

Reference(s):

1. Böger, P., B. Matthes, and J. Schmalfuss. 2000. Pest Manag. Sci. 56:497-508.

metham

methylcarbamodithioic acid

CAS # Acid: 144-54-7
Sodium salt: 137-42-8
Potassium salt: 137-41-7
Ammonium salt: 39680-90-5

26$^{(Z)}$

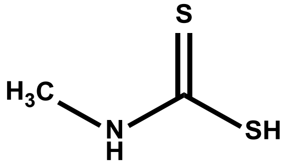
NOMENCLATURE

Common name: metham (BSI, ISO, WSSA)
Other name(s): metam; methylcarbamodithio acid; methyldithiocarbamic acid (IUPAC); sodium *N*-methyldithiocarbamate
Trade name(s): BUSAN; CARBAM; KARBATION; METACIDE 42; METAM; METAM 426; METAM CLR™; METAM KLR™; METHAM SODIUM; MAPOSOL; METILIDIENE K; NEMASOL; POLE FUME; RID-A-VEC®; RID-A-VEC® II; SISTAN; SOIL-PREP; VAPAM® HL SOIL FUMIGANT; VAPAM® RUP
Chemical family: dithiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

metham acid



Metham sodium salt

Molecular formula: *Acid:* $C_2H_5NS_2$; *NH_4 salt:* $C_2H_8N_2S_2$; *K salt:* $C_2H_4KNS_2$; *Na salt:* $C_2H_4NNaS_2$
Molecular weight: *Acid:* 107.19 g/mole; *NH_4 salt:* 124.22 g/mole; *K salt:* 145.28 g/mole; *Na salt:* 129.17 g/mole
Description: White crystalline solid as purified dry Na salt; orange to light yellow-green liquid with a sulfurous amine odor as the 42% w/w aqueous Na salt called the “manufacturers concentrate” (actual concentration varies from 42-50% w/w). Purified dry Na salt is extremely difficult to maintain (see Stability) and is virtually unavailable.
Density: *Acid:* NA; *Na salt:* NA; *42% w/w aqueous Na salt* 1.21 g/mL
Melting point: *Acid* NA; *Na salt* Decomposes before melting
Boiling point: *Acid:* NA; *Na salt:* Decomposes before boiling; *42% w/w aqueous Na salt* 110 C (1.02×10^5 Pa)
Vapor pressure: *42% w/w aqueous Na salt* 3.2×10^3 Pa (25 C)
Stability: Extremely hygroscopic and unstable as the dry Na salt; Stable in alkaline aqueous solution at concentrations above 20% w/v, but decomposes in acid solution to form ammonium ion and carbon disulfide.
Solubility:

Sodium salt
water 722,000 mg/L (20 C)
42% w/w aqueous sodium salt
water totally miscible
organic solvents (20 C):
acetone slightly miscible
ethanol moderately miscible
kerosene slightly miscible
xylene slightly miscible

pK_a: 4.9 (weak acid)
K_{ow}: *Acid:* NA; *Na salt:* 0.19 (pH 10)

HERBICIDAL USE

Metham is a soil fumigant applied to seedbeds to control weeds and soil-borne plant pathogens before planting. It can be applied in all crops, by soil injection at 142-356 kg ai/ha, by conventional sprayer at 178-356 kg ai/ha followed by immediate incorporation, through sprinkler irrigation systems at 267-356 kg ai/ha, through drip irrigation systems at 89-356 kg ai/ha, or through flood irrigation water at 178-356 kg ai/ha. A plastic tent or certain other soil coverings may be used to reduce volatility losses after application.

USE PRECAUTIONS

Fire hazard: Formulated products are aqueous and nonflammable; flash points are >93 C.
Corrosiveness: All formulated products corrode aluminum, copper, brass, and zinc. Corrosion rate for mild steel is 0.7 $mg/dm^2/d$, and for stainless steel is <0.2 $mg/dm^2/d$. May discolor iron, steel, and other metals.
Storage stability: Only slight decomposition after several years of storage in glass containers as an alkaline aqueous solution (381 g ai/L). Pure (solid) metham Na salt decomposes in several weeks. VAPAM is stable for up to 14 d at 50 C, and for >3.5 yr. at room temperature. METAM SODIUM crystallizes at -18 C and slowly re-dissolves upon warming. METAM 426 crystallizes at 0 C.
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: Avoid breathing vapors after application to soil. Flush skin or eyes immediately with running water; may be fatal if absorbed through skin.
Incompatibilities: Decomposes in acid solution; precipitates with metallic ions such as iron, aluminum, and copper.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Metham apparently is absorbed by plants as its breakdown product, methylisothiocyanate (MITC), suggesting that its action may be similar to dazomet. MITC may interact with nucleophilic centers, e.g. thiol groups, in enzymes and proteins (1). MITC also may inhibit activity of the Cu^{2+}-containing enzyme *o*-diphenoloxidase in potato and other organisms (2). These findings suggest that MITC may complex Cu necessary for *o*-diphenoloxidase activity and could complex other metals important to the activity of several enzymes. (more details on page 15)
Symptomology: Metham delays emergence or kills germinating seedlings before emergence from the soil. Dormant seeds or seeds with impermeable seed coats may not be killed by metham.
Absorption/translocation: Metham is not normally applied to foliage, but has some herbicidal activity when applied to

leaves. It is absorbed by tree roots, and translocated upward somewhat, where it kills vascular tissue.

Metabolism in plants: Metham is transformed rapidly to MITC, the phytotoxic molecule. Further metabolism is unknown.

Non-herbicidal biological properties: Metham is toxic to nematodes, fungi, bacteria, and insects in the soil.

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil

K_{oc}: Average is 10 mL/g (estimated) (3)

K_d: 0.02-0.08 mL/g

Transformation:

Photodegradation: Metham must be incorporated due to high volatility of its breakdown product, methylisothiocyanate (MITC); thus, there is little opportunity for photodegradation. Metham is subject to photolysis, however.

Other degradation: Degraded non-microbially in soil (assuming moisture is present) to MITC and sodium hydrogen sulfide. Under strong acid conditions, degradation to carbon disulfide and monomethylamine can occur.

Persistence: Extremely short persistence of 1-5 h in moist soil. Typical field half-life is 7 d. The primary breakdown product, MITC, disappears almost completely in 2-3 wks. Crop planting can begin 14-21 d after application except on soils high in clay or OM and where soil temperatures remain wet or cold (<15.6 C) following application.

Mobility: Both metham and MITC leach readily

Volatilization: Metham is not volatile, but its main breakdown product, MITC, is lost rapidly by volatility when applied to moist soil without incorporation.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with the 42% w/w aqueous technical grade metham sodium salt ("manufacturers concentrate") unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 812 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat, 2.28 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, yes; Eye irritation rabbit, mild.

VAPAM: Oral LD_{50} rat, 1294-1428 mg/kg; Dermal LD_{50} rabbit, 1012 mg/kg; 4-h inhalation LC_{50} rat, >4.7 mg/L; Skin irritation rabbit, severe; Skin sensitization guinea pig, yes; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOAEL 2.1 mg/kg/d; slight body weight reduction at 8.7 mg/kg/d; reductions in body weight and consumption of food and water, and histopathological lesions in nasal passages at 28.8 mg/kg/d

21-d dermal, rabbit: NOEL 31.25 mg/kg/d, systemic NOEL 125 mg/kg/d; slight to moderate erythema at 62.5 mg/kg/d; marked epidermal dermatitis at 125 mg/kg/d

Chronic toxicity: NA

Teratogenicity:

Rat: NOAEL 10 mg/kg/d; reduced body weight gain, reduced food intake, and effect on implantation at 40 and 120 mg/kg/d

Rabbit: NOAEL maternal 30 mg/kg/d, developmental 10 mg/kg/d; embryo lethality, neural tube defects, reduced maternal body weight gain and food intake at 100 mg/kg/d

Reproduction: NA

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: Chinese hamster bone marrow, not clastogenic; Human lymphocytes, some evidence of clastogenicity.

DNA damage/repair: UDS, negative

Wildlife:

METAM 426: Bobwhite quail oral LD_{50}, ~500 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck 8-d dietary LC_{50}, >5000 mg/kg; Bluegill sunfish 96-h LC_{50}, 0.39 mg/L; Rainbow trout 96-h LC_{50}, 0.079 mg/L

Use classification: Restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Carbonyl disulfide is reacted with methylamine and sodium hydroxide in water to produce metham sodium salt.

Purification of technical: NA

Analytical methods: Adding dilute cupric chloride solution to a dilute solution of metham produces a yellow color detectable by a spectrophotometer. Methyl isothiocyanate can be determined by GC.

Historical: Fumigating soil with metham was discovered in 1950 by Dorman and Lindquist. U.S. patent 2,766,554 was issued to Stauffer Chemical Company in 1956. Other Stauffer patents include U.S. patent 2,791,605 and British patent 789,690. VAPAM was first marketed in 1955 by Stauffer and later by Du Pont. Fungicidal properties of metham were first reported in 1951 (4) and again in 1956 (5).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Amvac; UAP-Platte; Taminco; UCB

Reference(s):

1. Cremlyn, R. J. 1991. Pages 303-304 *in* Agrochemicals: Preparation and Mode of Action. Wiley and Sons, New York. Vaughan and Ord. 1979. New Phytol. 83:361.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
3. Klopping, H. L. 1951. Thesis. University of Utrecht.
4. Overman and Burgis. 1956. Proc. Fla. St. Hortic. Soc. 69:250

methibenzuron

N-2-benzothiazolyl-N,N′-dimethylurea

CAS #: 18691-97-9

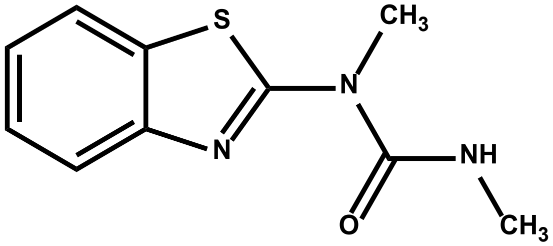
$7^{(C_2)}$

NOMENCLATURE

Common name: methibenzuron (WSSA)
Other names: methabenzthiazuron (E-ISO); BAY 74 283; S 25128; 1-(1,3-benzothiazol-2-yl)-1,3-dimethylurea (IUPAC); 1-benzothiazol-2-yl-1,3-dimethylurea (IUPAC)
Trade name(s): TRIBUNIL
Chemical family: substituted urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
methibenzuron



Molecular formula: $C_{10}H_{11}N_3OS$
Molecular weight: 221.28 g/mole
Description: Colorless odorless crystals
Density: NA
Melting point: 119-121 C
Boiling point: NA
Vapor pressure: 5.9×10^{-6} Pa (20 C)
Stability: Unstable in contact with strong acids or alkalis
Solubility: In water, 5.9 mg/L (20 C); acetone, 115.9 mg/L; methanol, 65.9 mg/L; hexane, 1-2 g/L
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 2.64

HERBICIDAL USE

Methibenzuron controls a broad spectrum of broadleaf weeds and grasses in cereals, legumes, maize, garlic, and onions. It is used with other herbicides for weed control in vineyards and orchards. Applied at rates of 1.4-2.8 kg a.i./ha. It is not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Non-corrosive
Storage stability: NA
Emergency exposure: Skin: wash affected area with soap and water; ingestion: give water and induce vomiting
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Chlorosis followed by necrosis of affected plant tissue
Absorption/translocation: Absorbed by roots and leaves; predominately xylem translocated
Metabolism in plants: Major metabolite is 1-hydroxymethyl-1-methyl-3-(benzothiazol)2-yl urea and its glucoside
Mechanism of resistance in weeds: Altered target site.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 527 mL/g
Persistence:
Lab experiments: DT_{50} > 1 yr at pH 4-9 (22 C)

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade methibenzuron unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, > 5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; non-irritating to skin or eyes (rabbits)
Chronic toxicity:
24-mo dietary, rats and mouse: NOEL 150 mg/kg diet
24-mo dietary, dog: NOEL 200 mg/kg diet
Wildlife:
Rainbow trout LC_{50} (96 h), 15.9 mg/L; Golden orfe, 29 mg/L; non-toxic to bees; Daphnia LC_{50} (48 h), 30.6 mg/L
Use classification: WHO class III; EPA (formulation) class IV

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

methiozolin

CAS #:: 403640-27-7

30$^{(R)}$

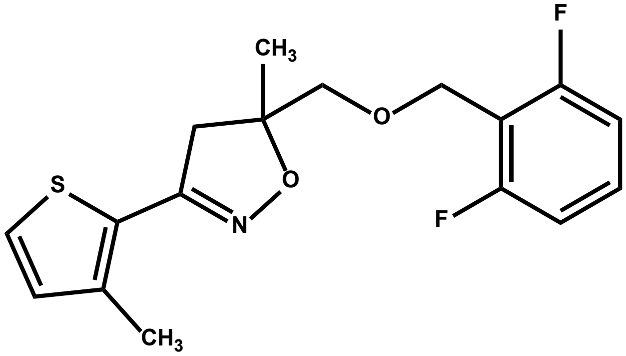
5-[[(2,6-difluorophenyl)methoxy]methyl]-4,5-dihydro-5-methyl-3-(3-methyl-2-thienyl)isoxazole

NOMENCLATURE

Common name: methiozolin
Other name(s): metiozolin; (5RS)-5-[(2,6-difluorobenzyloxy) methyl]-4,5-dihydro-5-methyl-3-(3-methyl-2-thienyl)-1,2-oxazole (IUPAC)
Trade name(s): POACURE™
Chemical family: Isoxazoline

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
methiozolin



Molecular formula: $C_{17}H_{17}F_2NO_2S$
Molecular weight: 337.38 g/mole
Description: NA
Density: NA
Melting point: 50.2 C
Boiling point: 402.7
Vapor pressure: NA
Stability: NA.
Solubility:
- water 3.4 mg/L (20 C)
- Acetone: 1000 mg/L
- Methanol:560 mg/L
- Hexane: 26 mg/L

pK_a: NA
K_{ow}: NA

HERBICIDAL USE

Methiozolin controls both annual and perennial biotypes of annual bluegrass by POST applications. Methiozolin has also PRE activity, thus provides residual control of annual bluegrass, crabgrasses (*Digitaria* sp.), and goosegrass (*Eleusine indica*).

USE PRECAUTIONS

Fire hazard: NA
Storage stability: NA.
Cleaning glassware/spray equipment: NA
Emergency exposure: NA.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Methiozolin inhibited root growth of corn, a susceptible grass ,at a very low dose with a GR50 of 0.03 μM. Using 14C-glucoseincorporation into corn root cell wall constituents, Lee et al[1].showed methiozolin inhibited biosynthesis of both cellulose and hemicellulose fractions greatly from 0.1 μM after 24 h of exposure. .However, the morphological symptoms did not resemble those of known cell wall synthesis inhibitors such as dichlobenil. Grossman et al.[2] suggested methiozolin might inhibit tyrosine aminotransferase. (more details on page 16)
Symptomology: Cessation of shoot and root growth without twisting, color change, burning, and other symptoms.[3]
Absorption/translocation: Methiozolin is primarily absorbed by the root system and translocated in the xylem. There is very limited phloem mobility.
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
- **Photodegradation:** NA
- **Other degradation:** NA.

Persistence: DT_{50} 49d (lab at 20C).
Field experiments: DT_{50} range 46.8 to 51.7 days
Mobility: NA
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Acute toxicity: >2500 mg/kg for rats;
Dermal LD50: >2500 mg/kg body wt for rats**.**
Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife:
HoneybeeLLD50 (48h) >100 ug/bee; Daphnia magna LC_{50} (48 h), 2.04mg/l; Fish LC_{50} (96 h): 1.53 mg/l; Algae EC_{50} (72 h):2.88 mg/l; Earthworms LC_{5}0 (14 d): >1000 mg/kg.
Use classification: Nontoxic

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: Discovered by Moghu Research Centre, Korea.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Moghu Research Centre, Korea.

Reference(s):

1. Grossmann, K., Hutzler, J., Tresch, S., Christiansen, N., Looser, R. and Ehrhardt, T. (2012), On the mode of action of the herbicides cinmethylin and 5-benzyloxymethyl-1, 2-isoxazolines: putative inhibitors of plant tyrosine aminotransferase. Pest. Manag. Sci., 68:482–492

metoxuron

CAS #: 19937-59-8 $5^{(C_1)}$

N’-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea

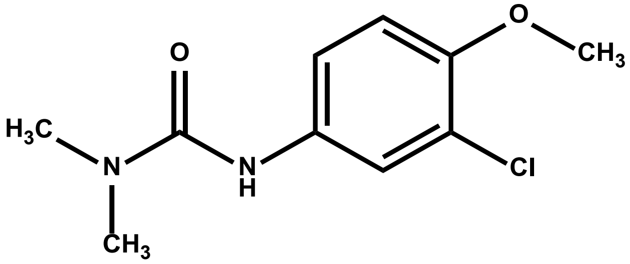
NOMENCLATURE

Common name: metoxuron
Other name(s): 3-(3-chloro-4-methoxyphenyl)-1,1-dimethylurea (IUPAC)
Trade name(s): DOSANEX®, DOSAFLO®
Chemical family: phenylurea; substituted urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

metoxuron



Molecular formula: $C_{10}H_{13}ClN_2O_2$
Molecular weight: 228.68 g/mole
Description: White liquid
Density: 0.8 g/mL (20 C)
Melting point: 126-127 C
Vapor pressure: 4.3×10^{-3} Pa
Stability: Stable (pH 4-9)
Solubility:
- water 678 mg/L (24 C)
- Practically insoluble:
- petroleum ether

pK$_a$: None (non-ionizable)
K$_{ow}$: log K_{ow} = 1.6

HERBICIDAL USE

Metoxuron is used preemergence and postemergence control of some grasses (*Agrostis spp.*, *Alopecurus myosuroides*, *Avena fatua* and *ludoviciana*, *Bromus sterilis*, *Lolium spp.*) and annual broadleaved weeds in winter wheat, winter barley, winter rye, some varieties of spring wheat, and carrots. Also used for haulm destruction in ware potatoes and pre-harvest defoliation in hemp, flax, and tomatoes.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable
Emergency exposure: Ingestation: Do not induce vomiting. Obtain medical attention as soon as possible.
Eye contact: Rinse immediately with gently running water for 15 min, keeping eyelids open. Obtain medical attention.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Usual photosynthesis inhibition symptoms
Absorption/translocation: Absorption by the leaves and roots, with translocation occurring primarily in the xylem
Metabolism in plants: Degradation in plants involves demethylation of the terminal nitrogen and hydrolysis of the urea moiety.
Mechanism of resistance in plants: Similar to other substituted urea herbicides

BEHAVIOR IN SOIL

Sorption:
K$_{oc}$: 120 mL/g
Transformation: Breakdown involves demethylation of the terminal nitrogen, further degradation to 3-chloro-4-methoxyaniline, ring hydroxylation, and ring cleavage
Persistence: Field dissipation DT_{50} = 10-30 d

TOXICOLOGICAL PROPERTIES

Acute toxicity:
Rat Oral LD_{50}, 3200 mg/kg; Dermal LD_{50}, >2000 mg/kg; Inhalation LC_{50}, >5 mg/L air
Subchronic toxicity:
NOEL rats(90 d), 1250 mg/kg/d; dogs 2500 mg/kg/d
Wildlife:
Avian toxicity: Oral LD_{50} chicks, 1250 mg/kg
Aquatic toxicity: LC_{50} rainbow trout, 18.9 mg/L (96 h); EC_{50} Daphnia magna, 26 mg/L (48 h); EC_{50} green algae, 0.064 mg/L; Oral LD_{50}, 850 mg/kg; LC_{50} earthworm, >1000 mg/kg soil
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

metribuzin

CAS #: 21087-64-9 $5^{(C_1)}$

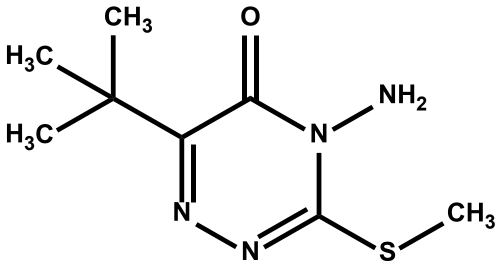
4-amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(4*H*)-one

NOMENCLATURE

Common name: metribuzin (BSI, ISO, WSSA)
Other name(s): BAY 6159H; BAY 6443H; BAY 94337; BAY DIC 1468; DPX 2504; metribuzine; 4-amino-6-*tert*-butyl-3-(methylthio)-*as*-triazine-5(4*H*)-one; 4-amino-6-*tert*-butyl-3-methylthio-1,2,4-triazin-5(4*H*)-one (IUPAC); 4-amino-6-*tert*-butyl-4,5-dihydro-3-methylthio-1,2,4-triazin-5-one (IUPAC)
Trade name(s): AXIOM®; CANOPY®; DOMAIN™ DF; FEINZIN®; GLORY; LEXONE®; METRIBUZIN 4; METRIBUZIN 75 DF; MISTRAL®; PYTHON®; SALUTE®; SENCOR® 4; SENCOR® DF 75; TURBO®
Chemical family: *as*-triazine; triazine; triazinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
metribuzin



Molecular formula: $C_8H_{14}N_4OS$
Molecular weight: 214.29 g/mole
Description: White crystalline solid, slight musty odor when pure; technical has a slight sulfurous odor
Density: 1.31 g/mL (20 C)
Melting point: 125.5-126.5 C
Boiling point: NA
Vapor pressure: 1.6×10^{-5} Pa (20 C); 2.7×10^{-2} Pa (60 C)
Stability: Relatively stable to heat and UV light; Stable at pH 4-9 (20 C)
Solubility:
water 1100 mg/L (20 C)
organic solvents g/100 mL (20 C):
acetone reaction possible
kerosene <0.8 benzene >20
methanol ~20 chloroform 127
methylene chloride >20
cyclohexanone 95 2-propanol 5-10
ethanol ~20 toluene 5-10
dimethyl formamide 16 xylene >20
n-hexane 0.05-0.1
pK$_a$: 1.0 (weak base)
K$_{ow}$: 44.7

HERBICIDAL USE

Metribuzin can be applied as follows: early preplant, PPI, PRE, or POST-directed (in certain states) at 0.28-0.84 kg ai/ha in soybeans; PRE or POST at 0.28-0.56 kg ai/ha in potatoes; at 0.28-1.12 kg ai/ha to established alfalfa and sainfoin; PRE and post-harvest at 0.56-2.24 kg ai/ha in asparagus; POST at 0.28 kg ai/ha in carrots; PRE at 0.28 kg ai/ha and POST at 0.094 kg ai/ha in field corn; PRE at 0.28-0.42 kg ai/ha in garbanzo beans, lentils, and dry field peas; POST at 0.14-0.21 kg ai/ha in lentils and spring peas; POST at 0.21-0.28 kg ai/ha in winter peas; PRE and POST at 0.84-5.6 kg ai/ha in sugarcane; PPI and POST at 0.28-1.12 kg ai/ha in tomatoes; and POST at 0.05-0.84 kg ai/ha in barley and winter wheat. Metribuzin controls many annual broadleaf weeds, including lambsquarters, pigweed spp., velvetleaf, jimsonweed, mustard spp., and common ragweed, along with certain annual grasses. It may be applied by conventional sprayer or impregnated on dry bulk fertilizer.

USE PRECAUTIONS

Fire hazard: The product SENCOR DF, SENCOR 75 SOLUPAK, and SENCOR 4 are non-flammable. SALUTE is non-flammable; flash point is 50.5 C. TURBO 8EC is non-flammable; flash point is 82.2 C.
Corrosiveness: All products are non-corrosive
Storage stability: Shelf life of all products is >2 yr. SENCOR 4 and TURBO 8EC become viscous at low temperatures. SALUTE crystallizes below 0 C, but the active ingredient re-dissolves at room temperature.
Cleaning glassware/spray equipment: Clean sprayers with water and detergent; clean pump, nozzles, and screens separately
Emergency exposure: Flush eyes with water for at least 15 min. Wash skin with soap and water. If SENCOR DF, SENCOR 75 SOLUPAK, SENCOR 4, or TURBO 8 are ingested, induce vomiting. If SALUTE 4 is ingested, do not induce vomiting; gastric lavage should be supervised by medical personnel because of possible lung damage from aspiration of the solvent.
Incompatibilities: Compatible with most liquid fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Susceptible weed seedlings emerge through treated soil but become chlorotic and completely necrotic (brown and desiccated) after 2 to 5 d in sunlight, often before they are large enough to be noticeable.
Absorption/translocation: Readily absorbed into roots by diffusion when soil-applied, and translocated readily in the xylem to the shoots. Uptake and translocation rates increase with higher transpiration rates. Metribuzin readily penetrates the symplasm but is not retained and leaches back into the apoplast. Uptake is moderate when foliar-applied, and translocation is acropetal. Downward movement in the phloem does not occur under normal conditions. Metribuzin

concentration in mature plants is highest in roots, stems, and leaves and is lowest in fruits and seeds.

Metabolism in plants: The most important detoxication reactions in soybeans are *N*-deamination, *N*-glucoside conjugation, and sulfoxidation followed by conjugation with homoglutathione. *N*-deamination probably is mediated by mixed function oxidase systems and results in deaminated (DA) metribuzin (4). *N*-deamination rate seems to correlate with metribuzin tolerance in soybean cultivars (5, 6). *N*-glucoside conjugation is mediated by metribuzin-*N*-glucosyl transferase. The resulting glucoside is conjugated rapidly with malonic acid to form the malonyl ß-*D*-(*N*-glucoside) conjugate. This two-step conjugation is the major detoxication pathway in tomato (7, 12). Sulfoxidation forms an unstable sulfoxide that is most commonly conjugated with homoglutathione. The sulfoxide also may undergo demethylthiolation to form diketo (DK) metribuzin. The DK metabolite can be conjugated with malonate, deaminated to form the deaminated diketo (DADK) metabolite, or can be incorporated into insoluble residues (8). Winter wheat metabolizes metribuzin to the DA, DADK, and DK derivatives (1).

Non-herbicidal biological properties: Several responses reported, but most appear to result from photosynthesis inhibition.

Mechanism of resistance in weeds: Metribuzin resistance has been identified in a biotype of redroot pigweed and attributed to reduced binding of metribuzin to its binding site on the D1 protein (10). Also, numerous species have developed biotypes resistant to triazine herbicides, usually through repeated use of atrazine and simazine. These biotypes are resistant to all *s*-triazines and also to the *as*-triazine metribuzin, although degree of metribuzin resistance may be somewhat less than the magnitude of *s*-triazine resistance.

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed on most soils. Metribuzin has high affinity for soil OM, but is less tightly adsorbed to clay. Adsorption decreases as soil pH increases (9, 11).

K_{oc} and K_d: Average K_{oc} is 60 mL/g (estimated) (13). Data for soils (25 C): K_{oc} 46.7 mL/g and K_d 0.246 mL/g for a sand with 1% OM and pH 4.3; K_{oc} 3.14 mL/g and K_d 0.0182 mL/g for a sandy loam with 1.1% OM and pH 6.6; K_{oc} 14.5 mL/g and K_d 0.221 mL/g for a silt loam with 2.9% OM and pH 5.9; K_{oc} 17 mL/g and K_d 0.196 mL/g for a clay loam with 2.2% OM and pH 6.4 mL/g

Transformation:

Photodegradation: Insignificant losses under field conditions. Rate constants under laboratory conditions were 0.05-0.28 per d on soil and 3.83 per d in water. Primary metabolites are the deaminated (DA), diketo (DK), and deaminated diketo (DADK) metabolites.

Other degradation: Microbial breakdown is the primary means of metribuzin dissipation from soils. Half-life is 172 and 439 d for a sandy loam under aerobic and anaerobic conditions, respectively. Primary metabolites are the DA, DK, and DADK metabolites. Non-microbial hydrolysis does not occur at 25 C and pH 5-9.

Persistence: Half-life typically is ~30-60 d during the growing season, but varies greatly (a few days to >4 mo) with soil characteristics and climatic conditions. Half-life under optimum degradation conditions usually is 14-28 d. Persistence is increased by cool temperatures or low soil moisture levels but metribuzin residues typically do not injure susceptible crops planted 1 yr after application. Rotation restrictions may apply, however, for root crops such as sugarbeets and onions.

Mobility: Readily leached in sandy soils low in OM content but has intermediate leaching potential on medium-texture soils, and is immobile on heavy soils high in OM. Higher pH increases metribuzin mobility. Metribuzin can move with soil runoff and is phytotoxic to algae and other aquatic plants. However, rapid photolysis in water greatly limits the impact of metribuzin in aquatic environments.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade metribuzin unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 1090 mg/kg; female rat, 1206 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50} rat, >0.65 mg/L; Skin irritation rat, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none

Subchronic toxicity:

Chronic toxicity:

24-mo dietary, rat: NOEL NA; no adverse effects at up to 100 mg/kg

12-mo dietary, dog: NOEL NA; no adverse effects at up to 100 mg/kg

Teratogenicity:

Rat: NOEL maternal <25 mg/kg/d, developmental <70 mg/kg/d; reduced placental weights, reduced fetal body weights, and increased incidence of delayed ossification at 200 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 30 mg/kg/d, developmental 85 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL maternal 30 mg/kg, developmental 750 mg/kg; reduced body weight gains in fetus; not a reproductive toxin

Mutagenicity: Not mutagenic in various tests

Wildlife:

Bobwhite quail oral LD_{50}, >168 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >100 mg/kg; 8-d dietary LC_{50}, >4000 mg/kg; Canary, red-winged blackbird, brownheaded cowbird, common grackle, and house sparrow oral LD_{50}, >100 mg/kg; Daphnia 48-h LC_{50}, 4.5 mg/L; Bluegill sunfish 96-h LC_{50}, 80 mg/L; Rainbow trout 96-h LC_{50}, 76 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Recrystallize from hexane/chloroform (4:1)

Analytical methods: Reflux with acetonitrile/water to release metribuzin and conjugated metabolites from plant tissue. Extracts are then filtered, the filtrate evaporated to drive off acetonitrile, and the water extract partitioned with chloroform. Metabolites are removed from the chloroform by aqueous base partitioning. The chloroform extract is cleaned-up on a Florisil column and analyzed by GC. The aqueous fraction containing metabolites is partitioned with chloroform buffered at pH 5 or is eluted through a C_{18} reverse phase column. The metabolite fraction is cleaned-up with a silica gel column and analyzed by GC. Detection limit for these analyses is 0.1 mg/kg or better.

Historical: The triazinone herbicide family was first described by Dornow et al. in 1964. Metribuzin was introduced in 1969 by Eue et al. Developed by Bayer CropScience AG and Du Pont Company; British patent 697,083 and German patent 1,795,784 were awarded to Bayer CropScience AG, and U.S. patent 3,905,801 to Du Pont. First reported in 1968 (2) and reviewed in 1972 (3). Commercial sale of metribuzin began in 1973 as SENCOR.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama**;** Bayer CropScience; DuPont Crop Protection

Reference(s):

1. Devlin, D. L. et al. 1987. Weed Sci. 35:741.
2. Draber, W. et al. 1968. Naturwissenschaften 55:446
3. Eue, L. 1972. Pfanzenschutz-Nachr. (Engl. Ed.) 25:175.
4. Fedtke, C. 1986. Pestic. Sci. 17:65.
5. Fedtke, C. 1991. Pestic. Sci. 31:175.
6. Fedtke and Schmidt. 1983. *In* J. Miyamoto and P. C. Kearney, eds., Pesticide Chemistry: Human Welfare and the Environment, Vol. 3. Pergamon Press, Oxford.
7. Frear, D. S. et al. 1983. Pestic. Biochem. Physiol. 19:270.
8. Frear, D. S. et al. 1985. Pestic. Biochem. Physiol. 23:56.
9. Ladlie, J. S. et al. 1976. Weed Sci. 24:505.
10. Oettmeier, W. et al. 1991. Pestic. Sci. 33:399.
11. Savage, K. E. 1976. Weed Sci. 24:525.
12. Stephenson, G. R. 1976. Weed Sci. 24:161.
13. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

metsulfuron-methyl

CAS #: 74223-64-6

$2^{(B)}$

methyl 2[[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino] carbonyl]amino]sulfonyl]benzoate

NOMENCLATURE

Common name: metsulfuron-methyl (ANSI, BSI, ISO, WSSA)

Other name(s): DPX-T6376; methyl 2-(4-methoxy-6-methyl-1,3,5-triazin-2-ylcarbamoylsulfamoyl)benzoic acid (IUPAC)

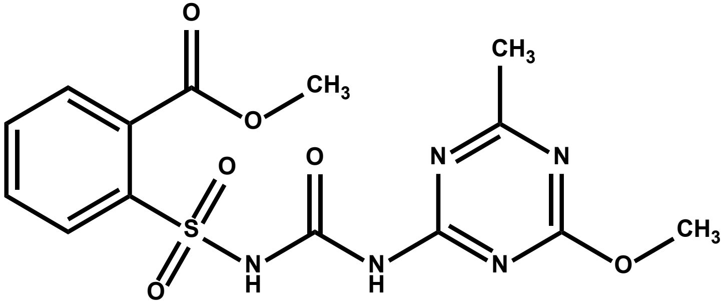
Trade name(s): ACCURATE™; ALLIE; ALLY® EXTRA; ALLY® XP; BRUSH-OFF; CANVAS®; CIMARRON®; CIMARRON® PLUS; CIMARRON® X-TRA; CIMARRON® X-TRA (MP); ESCORT® XP; FINESSE®; GROPPER; METSULFURON 60 EG; OUST® EXTRA; VALURON® 60DF

Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

metsulfuron-methyl



Molecular formula: $C_{14}H_{15}N_5O_6S$

Molecular weight: 381.36 g/mole.

Description: White to pale yellow solid, faint sweet ester-like odor

Density: 1.74 g/mL (25 C)

Melting point: 158 C

Boiling point: NA

Vapor pressure: 3.3×10^{-10} Pa; Henry's Law constant, 2.3×10^{-15} atm m^3/mole

Stability: Decomposes at 172 C

Solubility:

water (25 C), 548 mg/L (pH 5); 2790 mg/L (pH 7); 213,000 mg/L (pH 9)

organic solvents g/100 mL (20 C):

acetone 3.6	methanol 0.73
n-hexane 0.000079	methylene chloride 12.1

pK_a: 3.75 (25 C)

K_{ow}: 1 (pH 5); 0.018 (pH 7)

HERBICIDAL USE

Metsulfuron-methyl can be applied POST at 4.2 g ai/ha in wheat and barley for control of broadleaf weeds such as kochia, mustard spp., Russian thistle, and lambsquarters. It can be applied POST at 4.2 g ai/ha in grasses grown under the Conservation Reserve Program and at 4.2-12 g ai/ha in several pasture grass species.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are dry and non-flammable

Corrosiveness: Non-corrosive

Storage stability: Formulated products are stable if stored in an air tight container to keep free of moisture and high humidity.

Cleaning glassware/spray equipment: Wash glassware with detergent and water and then rinse with acetone. Rinse equipment with water followed by 0.5% v/v chlorine bleach.

Emergency exposure: Rinse eyes immediately with clean water for at least 15 min. and obtain urgent medical aid; if swallowed, wash out mouth with water

Incompatibilities: Compatible with most broadleaf herbicides and fungicides; tank mixing with highly acidic liquid fertilizers or with surfactants containing liquid fertilizers could cause crop injury, as could tank mixing with malathion or certain other organophosphate insecticides (especially when the crop is under stress at application); may be incompatible with additives that lower spray pH below 3.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Growth of treated plants is inhibited within hours after application, but injury symptoms usually appear >1-2 wk later. Meristematic areas gradually become chlorotic and necrotic, followed by a general foliar chlorosis and necrosis.

Absorption/translocation: Rapid foliar and root absorption. Metsulfuron-methyl translocates extensively in the xylem following root absorption, and less so in the phloem after foliar application. It accumulates in meristematic areas.

Metabolism in plants: Wheat and barley rapidly metabolize metsulfuron-methyl by hydroxylating the benzene ring at the #4 carbon followed by glucose conjugation at the ring hydroxyl group. Also detected were low levels of hydroxylation of the methyl group at carbon #6 on the triazine ring.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Sulfonylurea-resistant weed biotypes selected in the field by chlorsulfuron use typically are resistant to metsulfuron-methyl. The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: Low adsorption to clay, but greater adsorption to OM

K_{oc}: Average is 35 mL/g at pH 7 (4)

K_d: 1.4 mL/g for a Flanagan silt loam

Transformation:

Photodegradation: Negligible losses in the field

Other degradation: Microbial degradation is slow. Nonmicrobial hydrolysis is slow at high pH, but relatively rapid at lower pH. Hydrolysis cleaves the sulfonylurea bridge. Overall half-life varies from 1 wk to 1 mo, depending primarily on soil pH. Degradation rate increases with higher temperatures and higher soil moisture levels.

Persistence: Moderate residual with a typical half-life of 30 d (4), but ranging from 1-6 wk

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade metsulfuron-methyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.3 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

ALLY: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity:

28-d dietary, mouse: NOEL 7500 mg/kg; no histopathological effects

90-d dietary, rat: NOEL 1000 mg/kg; no histopathological effects

Chronic toxicity:

18-mo dietary, mouse: NOEL 5000 mg/kg; not oncogenic

24-mo dietary, rat: NOEL 500 mg/kg; not oncogenic; body weight effects at 5000 mg/kg

12-mo dietary, dog: NOEL male 500 mg/kg, female 5000 mg/kg

Teratogenicity:

Rat: NOEL 40 mg/kg/d; not teratogenic or embryotoxic; maternal toxicity at 250 mg/kg/d

Rabbit: NOEL 25 mg/kg/d; not teratogenic or embryotoxic; maternal toxicity at 100 mg/kg/d

Reproduction:

Rat: NOEL 500 mg/kg; body weight effects at 5000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: *In vitro* cytogenetics, weakly positive; *In vivo* cytogenetics, negative; Mouse micronucleus, negative

DNA damage/repair: Rat hepatocytes/UDS, negative.

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Honey bee topical LD_{50}, >25 μg/bee; Earthworm LC_{50} in soil, >1000 mg/kg; Daphnia 48-h LC_{50}, >12.5 mg/L; Bluegill sunfish 96-h LC_{50}, >150 mg/L; Rainbow trout 96-h LC_{50}, >150 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Product analysis and residues determined by HPLC (2).

Historical: Introduced by Du Pont Company; U.S. patent 4,370,480.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama, Arysta, Cheminova; DuPont Crop Protection

molinate

CAS #: 2212-67-1

$8^{(N)}$

S-ethyl hexahydro-1*H*-azepine-1-carbothioate

NOMENCLATURE

Common name: molinate (BSI, ISO, WSSA)

Other name(s): OMS-1373; R-4572; *S*-ethyl azepane-1-carbothioate (IUPAC); *S*-ethyl perhydroazepine-1-carbothioate (IUPAC); *S*-ethyl perhydroazepine-1-thiocarboxylate (IUPAC)

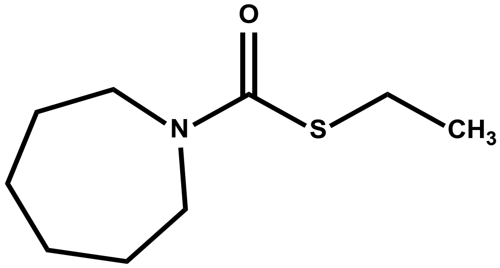
Trade name(s): ARROSOLO®; MOLINATE ESTRELLA; ORDRAM® 15-GM; ORDRAM® 8-E

Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

Molinate



Molecular formula: $C_9H_{17}NOS$

Molecular weight: 187.30 g/mole

Description: Clear bright-orange liquid, odor of decaying cabbage (characteristic of sulfur-containing compounds)

Density: 1.06 g/mL (20 C)

Melting point: NA (liquid at room temperature)

Boiling point: 136.5 C (1.33 x 10^3 Pa)

Vapor pressure: 7.46 x 10^{-1} Pa (25 C)

Stability: Stable at 120 C; photolysed in water DT_{50} 21 d (pH 7, 25 C)

Solubility: Stable for >1 mo at 100 or 120 C and for >2 yr at room temperature; Unstable in light

pK_a: None (non-ionizable)

K_{ow}: 756 (25 C)

HERBICIDAL USE

Molinate can be applied as follows: PPI, preflood at 3.36 kg ai/ha in water-seeded rice; POST, postflood at 3.36-5.6 kg ai/ha in water-seeded or drilled rice; PPI at 3.36-4.45 kg ai/ha in dry-seeded rice; POST, preflood at 2.24-3.36 kg ai/ha in dry- or water-seeded rice; and POST at flooding at 3.36 kg ai/ha by injection into irrigation water in dry-seeded rice. Molinate controls dayflower and certain annual grasses, such as barnyardgrass, sprangletop, and broadleaf signalgrass.

USE PRECAUTIONS

Fire hazard: Technical is non-flammable; flash point is >93 C. ORDRAM 8-E is non-flammable; flash point is 139 C (TOC) and fire point is 143 C.

Corrosiveness: Non-corrosive

Storage stability: Apparently indefinite storage life under ambient conditions.

Cleaning glassware/spray equipment: Wash glassware with acetone followed by water; Flush equipment with water.

Emergency exposure: If ingested, drink 1-2 glasses of water and induce vomiting. Atropine is antidotal.

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)

Symptomology: Germination is not inhibited, but growth of grass coleoptiles or broadleaf epicotyls ceases below the soil surface. Most susceptible plants fail to emerge. Emerging shoots may be distorted and twisted; leaves may remain tightly rolled in the whorl and fail to unroll normally. Injured dicot crops may have cupped or crinkled leaves with a thick, leathery texture. New leaves are puckered with a “drawstring” appearance.

Absorption/translocation: Readily absorbed by emerging shoots. Molinate is rapidly taken up by roots of tolerant plants and translocated to the leaves.

Metabolism in plants: CO_2 evolution results from hydrolysis and decarboxylation reactions on the alkyl or carbonyl groups of molinate applied in rice (3).

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

.

BEHAVIOR IN SOIL

Sorption: Adsorbed onto dry soil

K_{oc}: Average is 190 mL/g (5).

Transformation: Primarily degraded by microbes

Persistence: Half-life in most loam soils at 21-27 C is ~3 wk. Molinate residues do not persist long enough to injure susceptible crops planted 1 yr after application.

Mobility: Readily leaches in mineral soils, slightly more than EPTC.

Volatilization: Readily lost from wet soil surfaces when not incorporated immediately after application.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade molinate unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 720 mg/kg; mouse, 795 mg/kg; Dermal LD_{50} rat, 4000-4800 mg/kg; 4-h inhalation LC_{50} male rat, 0.00291 mg/L, female rat, 0.00139 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

ORDRAM 8-E: Oral LD_{50} male rat, 955 mg/kg, female rat, 599 mg/kg, mouse, 1260 mg/kg; Dermal LD_{50} rabbit, 3536 mg/kg; 4-h inhalation LC_{50}, 0.0616 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe

Subchronic toxicity:

90-d dietary, rat: NOEL 8 mg/kg/d

90-d dietary, dog: NOEL 20 mg/kg/d

Chronic toxicity: NA

Teratogenicity:

Rat: NOEL NA; not teratogenic

Reproduction:

Rat: NOEL NA; increased postnatal mortality at 3.2 mg/kg/d

Mutagenicity: Essentially non-genotoxic

Wildlife:

Mallard duck 5-d dietary LC_{50}, 13,000 mg/kg; Bluegill sunfish 96-h LC_{50}, 29 mg/L; Goldfish 96-h LC_{50}, 30 mg/L; Rainbow trout 96-h LC_{50}, 1.3 mg/L

ORDRAM 6E: Mallard duck 5-d dietary LC_{50}, 13,000 mg/kg; Mosquito fish 96-h LC_{50}, 26 mg/L.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Molinate can be separated from impurities on several columns and detected by GC with either thermal conductivity or flame ionization detectors.

Historical: Introduced by Stauffer Chemical Co.; U.S. patents 3,198,786 and 3,573,031.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Casida, J. E. et al. 1974. Science 184:573.
2. Fuerst, E. P. 1987. Weed Technol. 1:270.
3. Gray, R. A. 1965. Weeds 13:138.
4. Gronwald, J. W. 1991. Weed Sci. 39:435.
5. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

MSMA

Monosodium arsenate

CAS # Monosodium salt: 2163-80-6
Methylarsonic acid: 124-58-3

$27^{(Z)}$

NOMENCLATURE

Common name: MSMA (WSSA); MAA (methylarsonic acid) (WSSA) is the parent acid, methylarsonic acid

Other name(s): MAA = methylarsonic acid = parent acid of MSMA and DSMA (disodium salt); monosodium acid methanearsonate; sodium hydrogen methylarsonate (IUPAC)

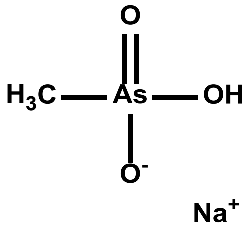
Trade name(s): ANSAR® 6.6; ARSONATE LIQUID; BUENO® 6; CHECK MATE; DACONATE 6; DACONATE® SUPER BRAND; MSMA 6.6; MSMA 6 PLUS; SUPERBRAND ARSONATE; MSMA 6 EC; TRIMEC® PLUS; MSMA PLUS; MSMA 6.6; MSMA 6 PLUS; MERGE 823; MESAMATE; SILVISAR; TRANS-VERT; WEED-E-RAD; WEEDHOE; 120 HERBICIDE

Chemical family: arsenical; organic arsenical

CHEMICAL AND PHYSICAL PROPERTIES

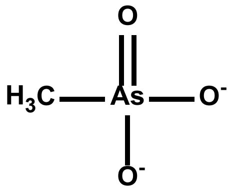
Chemical structure:

monosodium methane arsonate (MSMA)



$$\mathrm{H_3C{-}\underset{\underset{O^-}{|}}{\overset{\overset{O}{\|}}{As}}{-}OH}\qquad \mathrm{Na^+}$$

MAA



$$\mathrm{H_3C{-}\underset{\underset{O^-}{|}}{\overset{\overset{O}{\|}}{As}}{-}O^-}$$

Molecular formula: *MSMA*: CH_4AsNaO_3; *MAA:* CH_5AsO_3

Molecular weight: *MSMA*: 161.95 g/mole; *MAA:* 139.97 g/mole

Description: *MSMA*: Clear, odorless, light-yellow as a 51% w/v aqueous technical (purified dry technical is extremely difficult to maintain and is virtually unavailable); *MAA*: White crystalline solid as the purified dry technical.

Density: *MSMA*: 1.535 g/mL (25 C) for the 51% w/v aqueous technical, unknown for the pure dry technical; *MAA* 0.95 g/mL

Melting point: *MSMA*: (116-121 C) for the pure dry technical; *MAA* (161 C)

Boiling point: (110 ± 2 C) for the 51% w/v aqueous technical; unknown for the pure dry technical

Vapor pressure: *MSMA*: 1.33 x 10^{-3} Pa (20 C); *MAA* 9.99 x 10^{-6} Pa (25 C)

Stability: Dry purified technical is extremely hygroscopic and is unstable except in an anhydrous atmosphere.

Solubility:
MSMA
water 1,040,000 mg/L (25 C)
organic solvents g/100 mL (25 C):
n-hexane 0.00526
methanol 16
MAA
water 361,160 mg/L (25 C)

pK_a: 4.1 (1) and 9.02

K_{ow}: <1

HERBICIDAL USE

MSMA can be applied POST at 2.52 kg ai/ha in turf, POST at 2.22 kg ai/ha in cotton, and POST at 2.77 kg ai/ha in non-crop areas. Weeds controlled in turf include crabgrass spp., dallisgrass, and other grasses. MSMA also controls johnsongrass, nutsedge, foxtails, cocklebur, pigweeds, and others. A surfactant is required for satisfactory efficacy. The Ca salt formulation of methanearsonate (CALAR) was developed because of greater turf tolerance than MSMA.

USE PRECAUTIONS

Fire hazard: Formulated products are non- combustible

Corrosiveness: Formulated products are mildly corrosive.

Storage stability: Completely stable; solid formulations are somewhat hygroscopic and should be stored dry

Cleaning glassware/spray equipment: Flush with water

Emergency exposure: Wash eyes and skin with water for 15 min. If ingested, induce vomiting and lavage with water, followed by a saline cathartic, such as sodium sulfate. BAL (dimercaprol) is antidotal. Symptoms of mild poisoning include a salty taste, burning of throat, colicky stomach pains, and garlicky odor of breath or skin. Acute poisoning may occur with oral doses >30 g ai for an adult and symptoms include headache, vomiting, diarrhea, dizziness, stupor, convulsions, paralysis, and death.

Incompatibilities: Water high in Ca, Mg, and Fe may cause precipitation; these cations form insoluble methanearsonate salts.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood; rapid desiccation indicates cell membrane destruction

Symptomology: Foliar chlorosis and necrosis (desiccation)

Absorption/translocation: Readily absorbed by foliage and is translocated in the symplast. MSMA also is mobile in the apoplast; little translocation to shoots after root absorption from nutrient solution (5).

Metabolism in plants: Certain species metabolize MSMA to cacodylic acid. MSMA can be conjugated with sugars, amino acids, other organic acids, and other molecules. MSMA is not demethylated to form inorganic arsenicals and is not reduced to trivalent arsenic compounds in beans.

Non-herbicidal biological properties: Some fungicidal action; see U.S. Patent 3,106,509

Mechanism of resistance in weeds: Organical arsenical-resistant cocklebur biotypes have been reported (2), but the mechanism of resistance is unknown.

Sorption: Strongly adsorbed to soil; fixed by Fe and Al hydrous oxides in soil; sorption increases as size of clay fraction decreases.

K_{oc}: Average is 7000 mL/g (estimated) (5). Sand 250 mL/g; silty loam 2850 mL/g; silty clay 1170 mL/g; sandy loam 2190 mL/g

K_d: Sand 0.5 mL/g; silty loam 11.4 mL/g; silty clay 18.7 mL/g; sandy loam 39.4 mL/g

K_f: Sand 0.39 mL/g; silty loam 13.3 mL/g; silty clay 20 mL/g; sandy loam 34.8 mL/g

1/n: Sand 1.13; silty loam 0.695; silty clay 0.769; sandy loam 0.677

Transformation:

Photodegradation: Little to no losses when applied to soil; half-life was 990 d when irradiated on soil and 1155 d for the non-irradiated check; photolysis half-life is >30 d in water

Other degradation: Some breakdown by soil microbes; primarily degraded to arsenite with small amounts of cacodylic acid produced under aerobic laboratory conditions with a Hanford sandy loam

Persistence: Moderate to somewhat long residual with an average field half-life of 180 d (5)

Field experiments: In a Hanford fine sandy loam in the San Joaquin Valley of California under high irrigation, MSMA had a half-life of 55 d while its metabolite cacodylic acid had a half-life of 88 d.

Lab experiments: Isolated bacteria degraded 20% of applied MSMA in 11 d. Degradation was 0.8-12.5% after 160 d in both aerobic and anaerobic conditions.

Mobility: Medium to low mobility on sandy soil and is largely immobile on other soils. Even under heavy irrigation in a medium texture soil, MSMA primarily is found in the top 15 cm while its metabolite cacodylic acid is found only in the top 15 cm. MSMA did not leach in a Decatur clay loam, but leached to 51 cm in a Norfolk sandy loam.

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with dry technical grade methylarsonic acid (MAA) unless otherwise indicated.

Acute toxicity:

MSMA 51% w/v aqueous technical: Oral LD_{50} rat, 2833 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, 2.2 mg/L (male >2.23 mg/L, female 2.18 mg/L); Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

ARSONATE LIQUID: Oral LD_{50} rat, 1738 mg/kg; Dermal LD_{50} rabbit, 2500 mg/kg; 4-h inhalation LC_{50} rat, >20 mg/L; Skin irritation rabbit, mild; Eye irritation rabbit, mild **Subchronic toxicity:** NA

Chronic toxicity:

24-mo dietary, mouse: NOEL male 200 mg/mg, female 50 mg/mg; reduced body weight gain and increased water uptake at 400 mg/mg

12-mo dietary, dog: NOEL 2 mg/kg/d; diarrhea, vomiting, excessive salivation, and slightly decreased body weight at 35 mg/kg/d

Teratogenicity:

Rat: NOEL 10 mg/kg/d; slightly decreased food consumption and body weight gain at 100 mg/kg/d

Rabbit: NOEL 3 mg/kg/d; decreased food consumption and decreased body weight gain at 7 mg/kg/d**Reproduction:**

Rat: NOEL maternal 7 mg/kg/d, developmental 22 mg/kg/d; reduced body weight in males at 76 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative with or without metabolic activation; Mouse lymphoma, negative with or without metabolic activation

Structural chromosome aberration: CHO negative with or without metabolic activation

DNA damage/repair: Primary rat hepatocytes/ UDS, negative

Wildlife:

MSMA 51% w/v aqueous technical: Bobwhite quail oral LD_{50}, 425 mg/kg, 8-d dietary LC_{50}, 1667 mg/kg; Mallard duck 8-d dietary LC_{50}, >2866 mg/kg, 8-d dietary NOEC, 2866 mg/kg; Honey bee oral LD_{50}, 68 µg/bee, topical NOEL, 36 µg/bee; Daphnia 48-h LC_{50}, 77.5 mg/L, 48-h NOEC, 12.3 mg/L; Bluegill sunfish, 96-h LC_{50}, >51 mg/L, 96-h NOEC, 167 mg/L; Rainbow trout 96-h LC_{50}, >167 mg/L; 96-h NOEC, 167 mg/L

TARGET 6.6: Bobwhite quail oral LD_{50}, 834 mg/kg, 8-d dietary LC_{50}, 3269 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Honey bee oral LD_{50}, 68 µg/bee; Daphnia 48-h LC_{50}, 83 mg/L; Bluegill sunfish 96-h LC_{50}, >93.2 mg/L; Rainbow trout 96-h LC_{50}, >167 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: MSMA ($2CH_4AsNaO_3$) is produced from DSMA as follows:$2CH_3AsO(ONa)_2 + H_2SO_4 \rightarrow 2CH_4AsNaO_3 + Na_2SO_4$

Also, see Initial Scientific Review of MSMA/DSMA, December 1975, U.S. Environmental Protection Agency, and references 3 and 4. U.S. patents 2,889,347, 2,695,306, and 2,442,372.

Purification of technical: Recrystallization from methanol

Analytical methods: Titration with HCl, using an auto-end point titrometer; total arsenic determination is done with sulfuric/nitric acid digestion followed by reduction with potassium iodide and subsequent titration with iodine to the starch-iodine blue endpoint; atomic absorption spectrophotometry at 193.7 nm can be used. For residue methods, see Official Methods of Analysis, AOAC 12th ed., 25.006-25.013.

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Agriliance; Albaugh/Agri Star; Drexel; Helena; KMG Chemical; Monterey; PBI Gordon; PROKoZ;

Setre Chemical; UAP-Loveland Products; Verdicon (UAP-Professional Products)

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Haigler, W. E. et al. 1988. Weed Sci. 36:24.
3. Quick and Adams. 1919. Ind. Eng. Chem. 11:826.
4. Quick and Adams. 1922. J. Am. Chem. Soc. 44:805.
5. Sachs and Michael. 1971. Weed Sci.

monolinuron

CAS #: 1746-81-2 $7^{(C_2)}$

N′-(4-chlorophenyl)-*N*-methoxy-*N*-methylurea

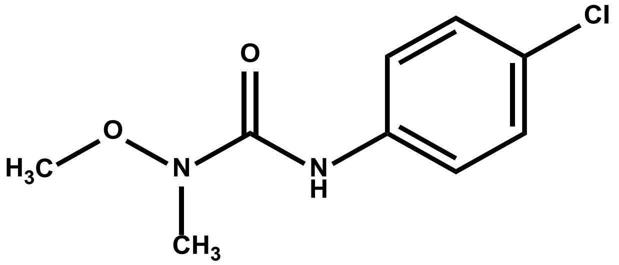
NOMENCLATURE

Common name: monolinuron (ISO)
Other name(s): AE F002747; HOE 002 747; 3-(4-chlorphenyl)-1-methoxy-1-methylurea (IUPAC)
Tradename(s): AFESIN®; ARESIN®
Chemical family: phenylurea, substituted urea, urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

monolinuron



Molecular formula: $C_9H_{11}ClN_2O_2$
Molecular weight: 214.65 g/mole
Description: Colorless crystals
Density: 1.3 g/mL (20 C)
Melting point: 80-83 C
Boiling point: NA
Vapor pressure: 1.3 x 10^{-3} Pa (22 C)
Stability: Stable in solution, but slowly decomposed in acidic and alkaline media; very stable in dry, neutral conditions; decomposes at 220 C
Solubility:
water, 735 mg/L (25 C)
readily soluble in common organic solvents
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 2.2

HERBICIDAL USE

Monolinuron is effective for annual broadleaf weeds including triazine-resistant biotypes and annual grass weeds. Used in soybean, white beans, yellow eye beans, kidney beans, lima sanpbeans, potatoes. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: Liquid formulations contain organic solvents that may be flammable.
Corrosiveness: Non-corrosive
Storage stability: Dry formulations are stable under normal storage conditions.
Cleaning glassware/spray equipment: Flush sprayer with water after removing nozzle tips and screens (clean tips and screens separately); clean glassware by detergent wash followed by acetone rinse
Emergency exposure: Eyes: Rinse with plenty of water. Skin: Rinse affected area with plenty of water. Ingestion: Rinse mouth with water, seek medical attention.

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Chlorosis and necrosis in affected plant tissue
Absorption/translocation: Absorbed by roots and leaves; translocated predominately in the xylem
Metabolism in plants: Not readily metabolized; selectivity achieved through placement
Mechanism of resistance in weeds: Altered site of action

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 250-500 mL/g
Transformation:
Photodegradation: Breaks down with exposure to ultraviolet light
Other degradation: Breakdown involves cleavage of the methyl and methoxy groups on the terminal nitrogen and simultaneous ring hydroxylation
Persistence:
Field experiments: DT_{50} 45-60 d
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >mg/kg; Dermal LD_{50} rabbit, >mg/kg
Wildlife: NA
Use classification: WHO class III; EPA (formulation) I

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

napropamide

N,*N*-diethyl-2-(1-naphthalenyloxy)propanamide

CAS # Racemic: 15299-99-7
R isomer: 41643-35-0
S isomer: 41643-36-1

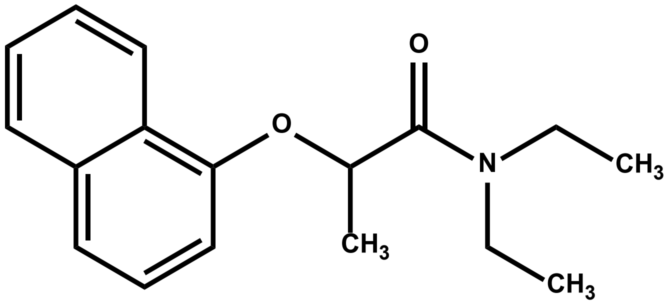
$15^{(K_3)}$

NOMENCLATURE

Common name: napropamide (BSI, ISO, WSSA)
Other name(s): R-7465; (*RS*)-*N*,*N*-diethyl-2-(1-naphthyloxy)propionamide (IUPAC); 2-(〈-naphthoxy)-*N*,*N*-diethyl-propionamide
Trade name(s): DEVRINOL
Chemical family: amide; substituted amide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
napropamide (RS)



Molecular formula: $C_{17}H_{21}NO_2$
Molecular weight: 271.36 g/mole
Description: White crystals (pure); brown solid (technical)
Density: NA
Melting point: 74.8-75.5 C (pure); 68-70 C (technical)
Boiling point: NA
Vapor pressure: 6.1×10^{-5} Pa (25 C); 1.3×10^{-2} Pa (50 C)
Stability: Decomposed by UV light; stable for at least 2 h in water; not decomposed at 40 C
Solubility:
water 73 mg/L (20 C)
organic solvents g/100 mL (20 C):

acetone > 100	kerosone 6.2
ethanol > 100	xylene 50.5
n-hexane 1.5	
4-methylpentan-2-one soluble	

pK_a: None (non-ionizable)
K_{ow}: 2100 (20 C); 2300 (25 C)

HERBICIDAL USE

Napropamide can be applied as follows: POST (but before weed emergence) at 4.48 kg ai/ha in artichokes, asparagus, and mint; PPI or PRE at 1.12-2.24 kg ai/ha in cole crops; PPI at 1.12-2.24 kg ai/ha in eggplant, peppers, and tomatoes; soil-applied (before weed emergence) at 3.36-16.8 in small fruits; PRE or POST at 1.12-2.24 kg ai/ha in tobacco; and soil-applied (before weed emergence) at 4.48 kg ai/ha in nut-bearing trees, citrus, and deciduoous and subtropical tree fruits. Napropamide controls many annual broadleaf and grass weeds including seedling perennial grasses.

USE PRECAUTIONS

Fire hazard: DEVRINOL 2-E is non-flammable; flash point is 191 C.
Corrosiveness: Non-corrosive
Storage stability: Stable for several years in packages
Cleaning glassware/spray equipment: Wash with acetone, then water. If acetone is not available, use hot soapy water.
Emergency exposure: If ingested, drink 1-2 glasses of water.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood. Napropamide inhibits growth by blocking the progression of dividing cells through the cell cycle into mitosis (5). Reduced rates of cell division and DNA synthesis occurred 12 and 8 h, respectively, after treatment, and apparently were due to a block in G_1 and G_2. This inhibitory effect may be due to an inhibition in the synthesis or activity of cell cycle specific proteins. Napropamide also inhibits alpha-amylase activity and the extent of this inhibition correlated with inhibition of tuber germination and subsequent shoot growth in purple nutsedge (7). (more details on page 14)
Symptomology: Susceptible seedlings typically fail to emerge. Napropamide primarily inhibits root growth, but also may inhibit shoot growth. In plants that emerge through treated soil, symptoms may include reduced root length, increased root diameter, and inhibition of lateral root growth, with root tips eventually becoming necrotic. Napropamide inhibits sprouting buds of purple nutsedge (7).
Absorption/translocation: Some foliar absorption occurs when applied POST, but napropamide is applied only to the soil. Napropamide was rapidly absorbed by tomato roots, and was translocated throughout the stems and leaves by 8 hr after application; little apoplastic movement from roots to shoots occurred in corn, however (2). Napropamide moves across the plasmalemma by passive diffusion (3). Napropamide selectivity seems to correlate with translocation rates among different species.
Metabolism in plants: Primary detoxification reactions in tolerant species such as tomatoes and fruit trees are *N*-dealkylation and ring hydroxylation (#4 carbon) followed by hexose conjugation (1, 6, 8). Metabolism appears to be the most important factor in napropamide selectivity.
Non-herbicidal biological properties: May have beneficial plant growth regulating effects on several crop species at sublethal concentrations (4).
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 700 mL/g (9)

Transformation:

Photodegradation: About 50% was lost by photodecomposition after 4-d on the soil surface during the summer. Under winter conditions the loss was ~30% in 8 d

Other degradation: Slowly degraded by soil microbes. In pure culture, a soil fungus metabolized napropamide rapidly (50% in 2 wk).

Persistence: Typical field half-life is 70 d (9). Half-life was 8-12 wk when incorporated in moist loamy sand and loam soils at 21-32 C.

Mobility: Only slightly leachable in most mineral soils. Napropamide leached ~2.5 cm in clay and silty clay soils, ~5 cm in loam, and 20 cm in loamy sand when 20 cm of water was applied in soil columns.

Volatilization: Little to no losses under field conditions.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade napropamide unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, >5000 mg/kg, female rat, 4680 mg/kg; Dermal LD_{50} rabbit, >4640 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA

DEVRINOL 10-G: Oral LD_{50} male rat, >5000 mg/kg

Subchronic toxicity:

90-d dietary, dog: NOEL 40 mg/kg/d

90-d dietary, rat: NOEL 30 mg/kg/d; reduced uterine weight in females at 40 mg/kg/d

Chronic toxicity:

18-d dietary, mouse: NOEL NA; decreased body weight gain; not carcinogenic

24-mo dietary, rat: NOEL 30 mg/kg/d; decreased body weight gain; not carcinogenic

Teratogenicity: NA

Reproduction: NA

Mutagenicity: Not mutagenic in three tests

Wildlife:

Bobwhite quail 7-d dietary LC_{50}, >5600 mg/kg; Honey bee oral LD_{50}, 121 μg/bee; Daphnia 48-h LC_{50}, 14.3 mg/L; Bluegill sunfish 96-h LC_{50}, 30 mg/L; Goldfish 96-h LC_{50}, >10 mg/L; Rainbow trout 96-h LC_{50}, 16.6 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React 2-(1-naphthoxy)-propionic acid with diethyl amine under dehydrating conditions.

Purification of technical: NA

Analytical methods: Extract soil and plants with acetone/ water followed by analysis with GC using a column of 5% SE-30 on 60.80 acid-washed Chromosorb W or other suitable column.

Historical: Introduced by Stauffer Chemical Company; U.S. patents 3,480-671 and 3,718,455.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): United Phosphorus

Reference(s):

1. Ashton, F.M. and A.S. Crafts. 1981. Mode of Action of Herbicides, 2^{nd} ed. John Wiley & Sons, New York.
2. Barrett and Ashton. 1981. Weed Sci. 29:697.
3. Barrett and Ashton. 1983. Weed Sci. 31:43.
4. Devlin, R. M. et al. 1982. Plant growth Regul. 1:113.
5. DiTomaso, J.M. et al. 1988. Pestic. Biochem. Physiol. 31:166.
6. Hatzios, K. K. and D. Penner. 1982. Metabolism of Herbicides in Higher Plants. Burgess Publ. Co., Minneapolis.
7. Mercado, L. R. 1975. Philippine Weed Sci. Bull. 2:19.
8. Murphy, J. J. et al. 1973. Weed Sci. 21:11.
9. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

naptalam

2-[(1-naphthalenylamino)carbonyl]benzoic acid

CAS # Acid: 132-66-1
Sodium salt: 132-67-2

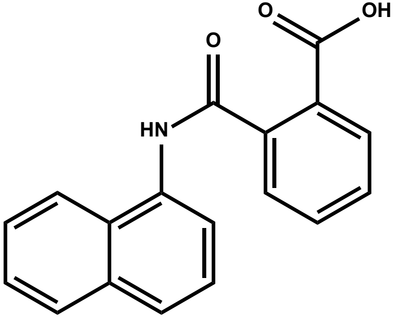
19$^{(P)}$

NOMENCLATURE

Common name: naptalam (BSI, ISO, WSSA)
Other name(s): ACP 322; NPA-3; sodium 2-[(1-naphthalenylamino)carbonyl]benzoate; *N*-1-naphthylphthalamic acid (IUPAC)
Trade name(s): ALANAP®; RESCUE®; NAPTALAMIE; NAPTRO
Chemical family: phthalamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
naptalam acid



Molecular formula: *Acid* $C_{18}H_{13}NO_3$; *Na salt* $C_{18}H_{12}NNaO_3$
Molecular weight: *Acid* 291.31 g/mole; *Na salt* 313.29 g/mole
Description: Purple crystalline solid, unpleasant odor
Density: *Acid* 1.36 g/mL; *Na salt* 1.39 g/mL
Melting point: 185 C
Boiling point: NA
Vapor pressure: <133 Pa (20 C)
Stability: NA
Solubility:

Acid
water 200 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 0.4
benzene insoluble
carbon tetrachloride 0.016
methylethyl ketone 0.3
dimethylformamide 3.72
xylene insoluble
DMSO 4.75
n-hexane insoluble
isopropanol 0.16

Sodium salt
water 249,000 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C):
acetone 1.34
benzene 0.044
dimethylformamide 4.75
methylethyl ketone 0.48
DMSO miscible
n-hexane insoluble
isopropanol 1.64
xylene 0.034

pK_a: 4.6 (weak acid)
K_{ow}: 1.06

HERBICIDAL USE

Naptalam can be applied as follows: PRE or POST at 2.2-4.5 kg ai/ha in cantaloupe, cucumber, muskmelon, and watermelon; preplant, PRE, or directed-POST at 4.5-9 kg ai/ha in various woody plants; PRE to at-cracking at 2.2-4.5 kg ai/ha in peanuts; and PRE to at-cracking or POST at 1.1-1.7 kg ai/ha in soybeans. Naptalam controls many annual broadleaf weeds including lambsquarters, common ragweed, cocklebur, redroot pigweed, and nightshade spp. Some grass weeds are controlled, including giant foxtail.

USE PRECAUTIONS

Fire hazard: ALANAP-L is non-flammable
Corrosiveness: ALANAP-L corrodes copper
Storage stability: Shelf life >4-5 yr. Active ingredient precipitates from ALANAP-L at -1 C, but warming with mild agitation redissolves the ai. Exposure of ALANAP-L to 60-65 C for >2 h can cause ring closure of the naptalam molecule, producing naptalam imide which precipitates.
Cleaning glassware/spray equipment: Wash and rinse with warm water. If naptalam has precipitated in the spray tank, several washes with ammonia may be required.
Incompatibilities: Low pH water could cause precipitation of naptalam acid. Extremely hard water or high electrolyte content may cause problems (spray nozzle blockage) in mixtures with liquid fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Not well understood. Naptalam appears to have both herbicidal and plant growth regulatory activity. It may function as an auxin-antagonist, perhaps by attaching to a phytotropin binding site and inhibiting auxin efflux from the basal ends of cells, thereby blocking basipetal auxin transport (1). Naptalam action appears to be similar to that of certain other amides (2). (more details on page 15)
Symptomology: Application to tomato foliage produces strong epinasty. Naptalam also produces an antigeotropic response, abolishing the normal curvature of roots toward the ground and of shoots toward light (1).
Absorption/translocation: Naptalam may accumulate somewhat in meristematic tissues, but mobility in both the apoplast (including xylem) and symplast (including phloem) appears to be limited.
Metabolism in plants: Rapidly metabolized to ⟨-naphthylamine and phthalic acid (3).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Poorly adsorbed to clay and OM
K_{oc}: Average is 20 mL/g (estimated) at pH 7 (4)
Transformation:

Photodegradation: Negligible losses

Other degradation: Slowly degraded by microbes

Persistence: Average field half-life is 14 d (4). About 3-8 wk of effective weed control from 4.5 kg ai/ha applied on a medium texture soil. Naptalam residues do not injure crops planted 1 yr after application.

Mobility: Leaches rapidly in coarse- or fine-textured soils. Heavy rains immediately after application can cause crop injury and reduced weed control. About 1.3 cm of rainfall is sufficient to activate a PRE application.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade naptalam acid unless otherwise indicated.

Acute toxicity:

Naptalam Na salt technical: Oral LD_{50} rat, 1770 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >2.1 mg/L; Skin irritation rabbit, mild; Skin sensitization, NA; Eye irritation rabbit, severe

ALANAP-L: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50} rat. >20 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, mild; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, rat: NOEL 50 mg/kg/d

90-d dietary, dog: NOEL 125 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL >714 mg/kg/d; not carcinogenic

24-mo dietary, rat: NOEL 30 mg/kg/d; not carcinogenic

12-mo dietary, dog: NOEL 5 mg/kg/d

Teratogenicity:

Rat: NOEL 115 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 150 mg/kg/d; no reproductive effects

Rabbit: NOEL 200 mg/kg/d; not teratogenic

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: *In vitro* cytogenetics, positive; Mouse micronucleus, negative

DNA damage/repair: Rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck oral LD_{50}, >4640 mg/kg, 8-d dietary LC_{50}, >10,000 mg/kg; Daphnia 48-h LC_{50}, 119 mg/L; Bluegill sunfish 96-h LC_{50}, 354 mg/L; Rainbow trout 96-h LC_{50}, 76.1 mg/L

ALANAP-L: Bobwhite quail 8-d dietary LC_{50}, >5620 mg/kg; Bluegill sunfish 96-h LC_{50}, 115 mg/L; Rainbow trout 96-h LC_{50}, 0.1 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Naptalam Na salt can be recrystallized from isopropanol.

Analytical methods: Naptalam is titrated by potentiometer with a standard acid and with nonaqueous perchloric acid; the difference determines the amount of phthalic acid. The first inflection point is between pH 9.5 and 8 and the second from pH 5.5 and 3. For extraction methods in several crops, see ref. 5.

Historical: Naptalam was discovered at Uniroyal Chemical Company in 1947; U.S. patents 2,556,664 and 2,556,665 issued to Uniroyal. The plant growth regulating activity of *N*-arylphthalamic acids was reported in 1949 (6). Naptalam was first registered and marketed in 1956 on cucumbers.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Uniroyal

Reference(s):

1. Corbett, J. R. et al. 1984. The Biochemical Mode of Action of Pesticides, 2nd ed. Academic Press, New York
2. Bromilow and Chamberlain. 1991. Pages 245-284 *in* R. C. Kirkwood, ed., Target Sites for Herbicide Action. Plenum Press, New York.
3. Ashton, F. M. and T. J. Monaco. 1991. Weed Science-Principles and Practices, 3rd ed. John Wiley & Sons, Inc., New York.
4. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
5. Lane, J. R. et al. 1958. J. Agric. Food Chem. 6:671.
6. Hoffman and Smith. 1949. Science 109:588.

nicosulfuron

CAS #: 111991-09-4 $2^{(B)}$

2-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-*N,N*-dimethyl-3-pyridinecarboxamide

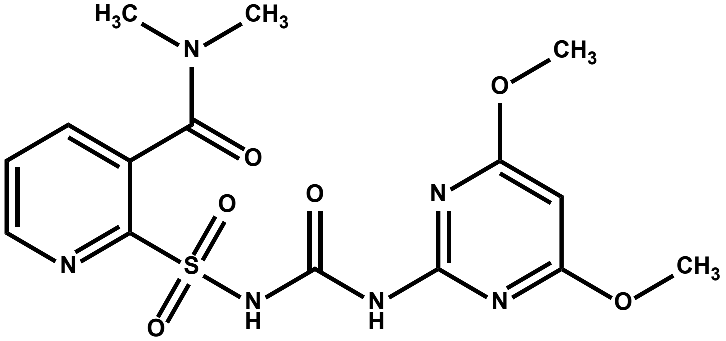
NOMENCLATURE

Common name: nicosulfuron (ANSI, ISO, WSSA)
Other name(s): DPX-V9360; HU-195; SL-950; 1-(4,6-dimethoxypyrimidin-2-yl)-3-(3-dimethylcarbamoyl-2-pyridylsulfonyl)urea (IUPAC); 2-(4,6-dimethoxy-pyrimidin-2-ylcarbamoylsulfamoyl)-*N,N*-dimethylnicotinamide (IUPAC)
Trade name(s): ACCENT®; ACCENT GOLD®WDG; BASIS® GOLD; CELEBRITY® PLUS; CLARION™; DPX-79406 75 DF; NICOSULFURON™ 75; STEADFAST®; STOUT®
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

nicosulfuron



Molecular formula: $C_{15}H_{18}N_6O_6S$
Molecular weight: 410.40 g/mole.
Description: White solid, phenolic odor
Density: 0.313 g/mL
Melting point: 141 - 144 C
Boiling point: NA
Vapor pressure: 1.6 x 10^{-14} Pa
Stability: Technical nicosulfuron and dry formulated products offered by Du Pont are stable > 2 years
Solubility:

water (25 C), 0.04% (pH 5); 1.2% (pH 7); 3.9% (pH 9)
organic solvents % (25 C):

acetone 1.8	ethanol 0.38
acetonitrile 2.3	*n*-hexane 0.04
chloroform 6.4	methylene chloride 16.0

pK_a: 4.3 (weak acid)
K_{ow}: 0.44 (pH 5); 0.018 (pH 7); 0.0068 (pH 9)

HERBICIDAL USE

Nicosulfuron can be applied POST at 17.5-70 g ai/ha alone and in mixtures in corn for control of most annual and some perennial grasses, including foxtail spp., shattercane, woolly cupgrass, wild-proso millet, johnsongrass, and quackgrass, as well as certain broadleaf weeds. A surfactant or oil adjuvant is required for efficacy with dry formulations~~maximum efficacy~~.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are dry and non-combustible
Corrosiveness: Technical and formulated products are non-corrosive
Storage stability: Stable under typical storage conditions
Cleaning glassware/spray equipment: Clean spray equipment with 1% v/v household ammonia (3% concentrate).
Emergency exposure: Wash skin with water. Flush eyes with water; call a physician if irritation persists. If ingested, consult a physician but intervention probably is not needed due to low toxicity.
Spray tank cleanout: Nicosulfuron, like most other commonly used herbicides must be thoroughly cleaned from the spray tank after each use. First, drain the tank, lines and booms and flush with clean water. Rinse all contaminated surfaces thoroughly. Fill the tank with clean water and add household ammonia at a rate of one gallon of 3% active for every 100 gallons of water. Flush ammonia solution through the lines, booms, and nozzles. Turn off the boom and top off the tank and circulate solution for 15 minutes. Flush hoses, boom and nozzles and drain the tank. Remove and clean nozzles, screens and strainers in a bucket of fresh cleaning solution. Repeat the operation. Drain tank and flush system with clean water several times.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth of treated plants is inhibited within a few h after application, but injury symptoms usually appear >1-2 wk later. Meristematic areas gradually become chlorotic and necrotic, followed by a general foliar chlorosis and necrosis.
Absorption/translocation: Nicosulfuron is rapidly absorbed by foliage and translocated to meristematic tissue. Nicosulfuron is usually-rainfast within 4 hours
Metabolism in plants: Mechanism for selectivity is due to differential metabolism. The half-life in corn is about 4.5 h whereas in sensitive plants half-life is several days. Generally, after 14 d residue levels are non-detectable in corn raw agricultural commodities. Major breakdown product is the pyridine sulfonamide.
Interactions: Nicosulfuron is reported to cause crop injury when applied—with systemic and foliarly applied organophosphate insecticides
Non-herbicidal biological properties: NA

BEHAVIOR IN SOIL

Sorption:

K_{oc} and K_d: Average K_{oc} is 30 mL/g at pH 6.5 (1). K_{oc} 38.4 mL/g and K_d 0.16 mL/g for a soil with 1.1% OM and pH 6.6; K_{oc} 28.8 mL/g and K_d 0.28 mL/g for a soil with 2.1%

OM and pH 6.5; K_{oc} 78.8 mL/g and K_d 1.73 mL/g for a soil with 4.3% OM and pH 5.4

Transformation: Nicosulfuron is rapidly degraded under aerobic conditions with a DT_{50} of about 26 d. Cleavage of the sulfonylurea bridge yields major degradation products. The rate of degradation of nicosulfuron was much reduced in sterilized soil. Under anaerobic conditions, the DT_{50} was approximately 6 mo (4).

Persistence: Average field half-life is ~21 d at pH 6.5 (1).

Field experiments: Half-lives were as follows: 0.75 mo for a soil with 1.3% OM and pH 5.5 at Stoneville, Mississippi; 0.25 mo for a soil with 1.4% OM and pH 6.0 at Newark, Delaware; 0.5 mo for a soil with 2.4% OM and pH 6.3 at Bradenton, Florida; 1 mo for a soil with 4.4% OM and pH 6.9 at Stettler, Alberta.

Mobility: Less than 0.001 mg/kg found below 50 cm after 5 annual applications at 70 g ai/ha indicating very low soil mobility.

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade nicosulfuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.9 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

ACCENT: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.6 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, mouse: NOEL 300 mg/kg/d

90-d dietary, rat: NOEL 20,000 mg/kg/d

90-d dietary, dog: NOEL 20,000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 7500 mg/kg/d not oncogenic

24-mo dietary, rat: NOEL 20,000 mg/kg/d not oncogenic

12-mo dietary, dog: NOEL male 5000 mg/kg/d, female 20,000 mg/kg/d; slight weight effect in males at 20,000 mg/kg/d

Teratogenicity:

Rat: NOEL 6000 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 100 mg/kg/d, fetal 500 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 5000 mg/kg; minimal decreases in weight gain and litter size at 20,000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: Mouse bone marrow/micronucleus, negative; Human lymphocytes/cytogenetics, negative

DNA damage/repair: Rat hepatocytes/UDS, negative; Rat liver/unspecified test, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Honey bee topical LD_{50}, >20µg/bee; Daphnia 48-h LC_{50}, >1000 mg/L; Bluegill sunfish 96-h LC_{50}, >1000 mg/L; Rainbow trout 96-h LC_{50}, >1000 mg/L

ACCENT: Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, >1000 mg/L; Bluegill sunfish 96-h LC_{50}, >1000 mg/L; Rainbow trout 96-h LC_{50}, >1000 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: U.S. patent 4,789,383 issued to Du Pont. Nicosulfuron was first marketed in 1991 as ACCENT.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection, Helm Agro, ISK Biosciences

norflurazon

CAS #: 27314-13-2

12$^{(F_1)}$

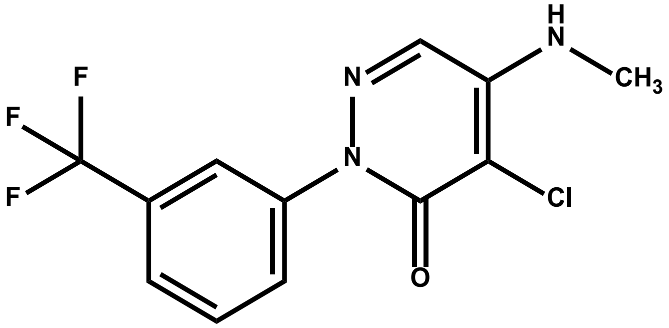
4-chloro-5-(methylamino)-2-[3-(trifluoromethyl)(phenyl)]-3(2*H*)-pyridazinone

NOMENCLATURE

Common name: norflurazon (ANSI, BSI, ISO, WSSA)
Other name(s): norflurazone; H-52143; SAN-9789H; 4-chloro-5-methylamino-2-(〈,〈,〈-trifluoro-*m*-tolyl)pyridazin-3-(2*H*)-one (IUPAC); 4-chloro-5-methyl-amino-2-(〈,〈,〈-trifluoro-*m*-tolyl)-3-(2*H*-pyridazinone; 4-chloro-5-methylamino-2-(〈,〈,〈-trifluoro-*m*-tolyl)-3-(2*H*)-pyridazinone
Trade name(s): ZORIAL®; PREDICT®; SOLICAM®
Chemical family: fluorinated pyridazinone; pyridazinone; phenylpyridazinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *norflurazon*



Molecular formula: $C_{12}H_9ClF_3N_3O$
Molecular weight: 303.67 g/mole
Description: Crystalline powder, white to grayish brown
Density: 0.63 g/mL (20 C)
Melting point: 177 ± 3 C
Boiling point: NA
Vapor pressure: 2.67 x 10^{-6} Pa (20 C); 3.87 x 10^{-6} Pa (25 C); 3.33 x 10^{-5} Pa (40 C); 3.33 x 10^{-4} Pa (60 C); 2.40 x 10^{-3} Pa (80 C); 1.33 x 10^{-2} Pa (100 C)
Stability: Stable after 4 wk at 50 C or 15 d at 70 C; moderately photostable
Solubility:
water 28 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 5
carbon disulfide insoluble
ethanol 14.2
xylol 0.25
pK_a: None (non-ionizable)
K_{ow}: 280 ± 15 (25 C)

HERBICIDAL USE

Norflurazon can be applied as follows: PRE at 3.36-4.5 kg ai/ha in tree, nut, and vine crops (almonds, apples, apricots, avocados, blackberries, blueberries, cherries, etc.); PRE at 2.24-4.5 kg ai/ha in hops and for industrial vegetation management (rights-of-way, tank storage sites, utility installations, etc.); PRE at up to 9 kg ai/ha in irrigated citrus and PRE at up to 4.5 kg ai/ha in non-irrigated citrus; PRE at 1.12-2.24 kg ai/ha in soybeans; PRE at 0.56-2.24 kg ai/ha in cotton; PRE at 1.34-1.61 kg ai/ha in peanuts; and PRE at 3.36 kg ai/ha in ornamentals. Norflurazon controls many grasses and sedges such as crabgrass spp., barnyardgrass, foxtail spp., and spikrush, as well as many broadleaf weeds including prickly sida, purslane, Russian thistle, and shepherd's purse.

USE PRECAUTIONS

Fire hazard: Technical and all formulated products are non-flammable. SOLICAM and ZORIAL are combustible.
Corrosiveness: Technical and all formulated products are non-corrosive.
Storage stability: Stable for >1 yr at room temperature.
Cleaning glassware/spray equipment: NA
Emergency exposure: Induce vomiting if ingested and seek medical attention. Flush eyes with water. Wash skin with soap and water. See a doctor if eye or skin irritation persists. No antidote is known.
Incompatibilities: Compatible with hard water.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme phytoene desaturase in the carotenoid biosynthesis pathway (more details on page 14)
Symptomology: Interveinal whitening of leaf and stem tissue becomes apparent as susceptible seedlings emerge from soil. Growth may continue for several days, but seedlings lack green photosynthetic tissue and soon become necrotic.
Absorption/translocation: Absorbed readily into roots by diffusion and translocated acropetally in the xylem
Metabolism in plants: Desmethyl norflurazon is a major metabolite in alfalfa.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Absorbed by clay and OM; application rate is determined by clay and OM content.

K_{oc} and K_d; Average K_{oc} is 700 mL/g (2). K_d 940 mL/g and K_d 17 mL/g with norflurazon applied at 0.07 mg/kg, and K_{oc} 290 mL/g and K_d 5.2 mL/g with norflurazon at 7 mg/kg in a clay loam; K_{oc} 750 mL/g and K_d 4.5 mL/g with norflurazon applied at 0.07 mg/kg; K_{oc} 270 mL/g and K_d 1.4 mL/g with norflurazon at 7 mg/kg in a sandy loam; K_{oc} 570 mL/g and K_d 4.0 mL/g with norflurazon applied at 0.07 mg/kg; and K_{oc} 290 mL/g and K_d 2.0 mL/g with norflurazon at 7 mg/kg in a silt loam; K_{oc} 160 mL/g and K_d 0.93 mL/g with norflurazon applied at 0.07 mg/kg; and K_{oc} 110 mL/g and K_d 0.65 mL/g with norflurazon at 7 mg/kg in sand

K_f: 7.11 mL/g for a clay loam; 2.37 mL/g for a sandy loam; 2.51 mL/g for a silt loam; and 0.716 mL/g for a sand.

Transformation:

Photodegration: Half-life is 1.04 ± 0.05 h in water with deschloro-norflurazon and small amounts of other products formed. Half-life is 21.17 ± 0.75 d for norflurazon applied at 542 mg/kg on a silt loam at 25 C with metal halide lamps supplying 155.1 W/m^2 average light intensity (equivalent to a half-life of 41 d with full-noon-day sun in Cincinnati); desmethyl norflurazon, CO_2, and small amounts of other products were formed. Photodegradation contributes significantly to field dissipation when norflurazon remains on the surface.

Other degradation: Half-life is ~ 130 d for aerobic degradation in soil with CO_2 and desmethyl norflurazon as major metabolites. Half-life is ~6-8 mo in aerobic aquatic conditions with desmethyl norflurazon as the major and CO_2 as the minor (~1%) metabolites. Half-life is ~8 mo in aerobic anaerobic aquatic conditions with desmethyl norflurazon as the major and CO_2 as the minor (~8%) metabolites.

Persistence: Moderate to long residual with a half-life of 45-180 d (varies with clay and OM content) when applied at recommended rates in soils from the Mississippi Delta and southeastern U.S.

Mobility: Norflurazon does not leach appreciably, but OM and clay content are determining factors. Losses in soil runoff water are very limited (1).

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade norflurazon unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 9000 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none.

ZORIAL RAPID 80 DF: Oral LD_{50} rat, 1140 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg;p 4-h inhalation LC_{50} rat, >200 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild.

Subchronic toxicity:

90-d dietary, rat: NOEL male 21 mg/kg/d; increased thyroid size.

90-d dietary,dog: NOEL 12.7 mg/kg/d; emesis, soft stools.

Chronic toxicity:

24-mo dietary, mouse: NOEL 41 mg/kg/d (340 mg/kg), liver hyperplasia/hypertrophy, hepatoma.**24-mo dietary rat:** NOEL 19 mg/kg/d (375 mg/kg); accelerated aging changes

12-mo dietary dog: NOEL 16 mg/kg/d (50 mg/kg)

6-mo dietary dog: NOEL 3.75 mg/kg/d (150 mg/kg); increased liver weight; increased colloidal vacuole in thyroid.

Teratogenicity:

Rat: NOEL 400 mg/kg/d; reduced maternal weight gain

Rabbit: NOEL 10 mg/kg/d; maternal weight decreased; delayed skeletal development

Reproduction:

Rat: NOEL 75 mg/kg/d (150 mg/kg); increased liver weight in pups.

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Negative

DNA damage/repair: UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >1250 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Honey bee oral LD_{50}, 235 μg/bee, topical LD_{50}, >236 μg/bee; Daphnia 48-h LC_{50}, >15 mg/L; Bluegill sunfish 96-h LC_{50}, 16.3 mg/L; Rainbow trout 96-h LC_{50}, 8.1 mg/L

ZORIAL RAPID 80: Rainbow trout 96-h LC_{50}, 6 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Trifluoromethylaniline is acidified, then nitrited, followed by reaction with sulfites, and then by acidification to form the hydrazine hydrochloride which is reacted with mucochloric acid. The brown oil is then reacted with monomethylamine, forming a fine suspension. Base is then added and solvents distilled off. The norflurazon suspension is filtered and washed. See U.S. patent 3,644.355.

Purification of technical: Two or three successive recrystallizations from acetone with cooling.**Analytical methods:** Formulated products can be assayed for norflurazon by GC using FID and a diphenyl phthalate internal standard. Norflurazon and its desmethyl metabolite can be determined in soil samples by extraction with KOH/methanol/water using heat and shaking, and in water samples by dilution with methanol. The methanol/water is partitioned with pentane, diluted with additional water, and extracted with methylene chloride. After solvent exchange to toluene, norflurazon is quantified by GC-ECD. Norflurazon and its desmethyl metabolite can be determined in tissue samples by blending the sample in 0.5 N KOH and hydrolyzing for 1 h at 90-95 C. The hydrolysate is cooled and methanol is added. The sample is shaken, filtered, and an aliquot extracted with dichloromethane. The dichloromethane is then evaporated and the sample taken up in water, cleaned-up with C18 Solid-phase extraction, and quantified by GC-ECD using a methyl silicone wide-bore capillary column. Norflurazon and its desmethyl metabolite can be determined in crop samples by extracting with methanol (samples with <10% oil) or with 2:1 acetone/methanol (samples with >10% oil). Aqueous NaCl (5%) is added to the extract which is then partitioned with pentane. The aqueous fraction is further diluted with additional 5% NaCl and extracted with methylene chloride. After solvent exchange to toluene, norflurazon and the desmethyl metabolite are quantified by GC-ECD (SAI AM-0806).

Historical: First synthesized by C. Ebner and M. Schuler in Belgium. Norflurazon was introduced by Sandoz Ag in 1968; U.S. patent 3.644,355.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Southwick, L. M. et al. 1993. J. Agric. Food Chem. 41:1503.
2. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1

oryzalin

4-(dipropylamino)-3,5-dinitrobenzenesulfonamide

CAS #: 19044-88-3

$3^{(K_1)}$

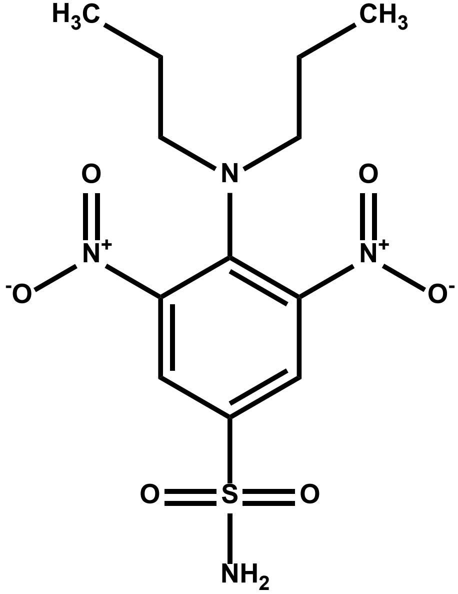
NOMENCLATURE

Common name: oryzalin (ANSI, BSI, ISO, WSSA)
Other name(s): ELI-119; 3,5-dinitro-N^4,N^4-dipropylsulfanilamide (IUPAC)
Trade name(s): ORYZALIN 4 A.S.; SURFLAN®; DIRIMAL; RYCLEAN; RYZELAN; RYZELON; WEED STOPPER; ROUT®; XL 2G
Chemical family: dinitroaniline

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

oryzalin



Molecular formula: $C_{12}H_{18}N_4O_6S$
Molecular weight: 346.36 g/mole
Description: Bright-orange crystalline powder, odorless
Density: NA
Melting point: 141-142 C
Boiling point: Decomposes at 265 C
Vapor pressure: <1.33 x 10^{-6} Pa (25 C)
Stability: Decomposed by UV light
Solubility:
water 2.6 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone >50
acetonitrile >15
benzene 0.4
dichloromethane >3
ethanol soluble
methanol >5
methyl cellosolve >50
xylene 0.2
pK_a: 9.4
K_{ow}: 5420 at pH 7

HERBICIDAL USE

Oryzalin can be soil-applied (before weed emergence) at 2.24-6.72 kg ai/ha on non-bearing fruit and nut crops, vineyards, rights-of-way, or at 2.24-4.48 kg ai/ha in Christmas tree plantations and landscape nurseries.

It controls many annual grasses and broadleaf weeds, including barnyardgrass, annual bluegrass, crabgrass spp., foxtail spp., fall panicum, field sandbur, carpetweed, common chickweed, lambsquarters, and pigweed spp. Oryzalin can be applied by conventional sprayer in water or mixed with liquid fertilizer, and via chemigation.

USE PRECAUTIONS

Fire hazard: Technical oryzalin is a flammable solid. SURFLAN A.S. is aqueous and non-flammable.
Corrosiveness: Non-corrosive
Storage stability: NA
Cleaning glassware/spray equipment: Clean equipment with detergent and water
Emergency exposure: If SURFLAN is ingested, do not induce vomiting; administer 6-8 teaspoons activated charcoal and a large quantity of water.
Incompatibilities: Compatible with most fertilizers and other wettable powder and liquid pesticide formulations, if not highly alkaline. Oryzalin products are compatible with hard water.

BEHAVIOR IN PLANTS

Mechanism of action: Mitotic disruption through inhibition of the microtubule protein tubulin (more details on page 12)
Symptomology: Most susceptible annual grasses and small-seeded broadleaf weeds fail to emerge, due to inhibition of coleoptile growth or hypocotyl unhooking. Seed germination is not inhibited. Root growth inhibition is a prominent symptom on emerged seedlings and established plants, especially in development of lateral and secondary roots. Roots appear stubby with tips becoming thickened. Grass stems such as corn may be purple near the base. The base of grass shoots swell, appearing bulbous, and the hypocotyl may swell in broadleaves. Shoots may be deformed and brittle.
Absorption/translocation: Oryzalin is soil-applied and is thought to be absorbed by roots and coleoptiles. Kinetics of oryzalin uptake suggest its accumulation in cells at concentrations much higher than in the external solution, but this does not appear to be an energy requiring process (5). Oryzalin is strongly lipophilic and rapidly partitions into membranes and other lipid components of root tissue. Consequently, it is not considered to translocate to any degree.
Metabolism in plants: Following soil application of oryzalin, no significant terminal residues or specific oryzalin metabolites were detected in either seed or forage of soybeans (2). Furthermore, carbon derived from oryzalin metabolism was incorporated into a variety of plant constituents.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Trifluralin-resistant

goosegrass from the southern U.S.is resistant to other dinitroaniline herbicides, including oryzalin (4). The resistance mechanism may involve either a change in the binding site on tubulin subunits (6) or an altered microtubule-associated protein (7).

BEHAVIOR IN SOIL

Sorption: Soil OM and clay content influence the required application rate.

K_{oc}: Average is 600 mL/g (9), but ranges from 93-2700 mL/g

Transformation:

Photodegradation: Photodecomposition has been demonstrated in lab studies

Other degradation: Microbes probably degrade oryzalin. No specific soil organism has been identified as responsible for the degradation.

Persistence: Short to moderate residual with a typical field half-life of 20 d (9). Field half-life may range fro 20-128 d.

Mobility: Limited leaching under natural rainfall conditions.

Volatilization: Minimal losses that do not reduce the efficacy of oryzalin applied without incorporation

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade oryzalin unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat and mouse, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >3 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

SURFLAN A.S.: Oral LD_{50} rat, >500 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 1-h inhalation LC_{50} rat, >0.5 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, dog: NOEL 18.75 mg/kg/d

Chronic toxicity:

24-mo dietary mouse: NOEL 100 mg/kg/d; no effects at up to 71 mg/kg/d; not oncogenic at up to 522 mg/kg/d; not carcinogenic

24-mo dietary, rat: NOEL 14 mg/kg/d; considered a Class C oncogen because of increased incidence of thyroid tumors (considered a result of the anti-thyroxin properties of oryzalin), an equivocal increase in incidence of skin tumors, and an increased incidence of mammary tumors

Teratogenicity:

Rat: NOEL 50 mg/kg/d; not teratogenic

Rabbit: NOAEL 125 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL NA, not a reproductive toxin at 112 mg/kg/d

Mutagenicity: Negative in several tests; positive for intraperitoned administration of oryzalin in hamster/SCE test (negative for oral administration)

Wildlife:

Bobwhite quail oral LD_{50}, 506.7 mg/kg; Mallard duck oral LD_{50}, >50 mg/kg; Chicken oral LD_{50}, 1000 mg/kg; Honey bee oral LD_{50}, 11 μg/bee; Bluegill sunfish 96-h LC_{50}, 2.88 mg/L; Goldfish fingerling 96-h LC_{50}, >1.4 mg/L; Rainbow trout 96-h LC_{50}, 3.26 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Recrystallize from acetone-petroleum ethers

Analytical methods: In formulated products, absorption of the bright orange solution of oryzalin in benzene; ethyl acetate is measured at 383 nm after removal of colored impurities. Alternatively, the sample can be extracted with acetonitrile, and oryzalin concentration determined by reverse-phase HPLC. Residue determination requires extraction of crop tissue or soil with a solvent such as methanol, solvent partitioning, conversion of oryzalin to its dimethyl derivative with methyl iodide, and removal of interfering substances on an alumina column. Final measurement is made GC with electron affinity detection. Test sensitivity is 25-50 μg/kg (1).

Historical: First reported in 1969 with a description of herbicidal properties (3); introduced in Bulgaria in 1973 by Eli Lilly & Company; U.S. patent 3,367,949 was issued February 6, 1968

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Adama; Dow AgroSciences; Helena; Monterey; Scotts

Reference(s):

1. Decker and Johnson. 1976. Pages 433-ff in G. Zweig and J. Sherma, eds., Analytical Methods for Pesticides and Plant Growth Regulators, Vol. 8. Academic Press, New York.
2. Golab, T. et al. 1975. Pestic. Biochem. Physiol. 5:196.
3. Gramlich, J. V. et al. 1969. Abstr. Weed. Sci. Soc. Am. 22.
4. Mudge, L. C. et al. 1984. Weed Sci. 32:591.
5. Upadhyaya and Nooden. 1980. Plant Physiol. 66:1048.
6. Vaughn, K. C. et al. 1987. Plant Physiol. 83:956.
7. Vaughn, K. C. et al. 1990. Weed Technol. 4:157.
8. Vaughn and Lehnen. 1991. Weed Sci. 39:450.
9. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

oxadiargyl

CAS #: 39807-15-3

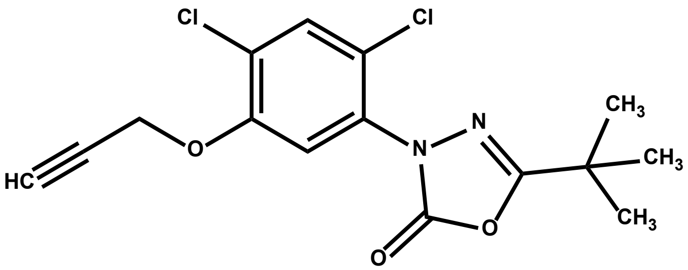
3-[2,4-dichloro-5-(20propynyloxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3*H*)-one

NOMENCLATURE

Common name: oxadiargyl (ISO proposed)
Other name(s): RP-020630; 5-*tert*-butyl-3-[2,4-dichloro-5-(prop-2-ynyloxy)phenyl]-1,3,4-oxadiazol-2(3*H*)-one (IUPAC)
Trade name(s): RAFT®; TOPSTAR®; CARIOCA®
Chemical family: oxadiazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
oxadiargyl



Molecular formula: $C_{15}H_{14}Cl_2N_2O_3$
Molecular weight: 341.2 g/mole
Description: Odorless, white powder with little agglomerates
Density: 1.48 g/mole (20 C)
Melting point: 131 C
Boiling point: NA
Vapor pressure: 2.5 x 10^{-6} Pa
Stability: Stable
Solubility: water 0.37 mg/L (20 C)
pK$_a$: NA
K$_{ow}$: log K_{ow} = 3.95

HERBICIDAL USE

Oxadiargyl is used PRE at 50 to 150 g ai/ha in transplanted, dry direct seeded and water seeded rice and in winter wheat and provides effective control of many annual monocotyledenous and dicotyledonous weeds (1). Development is also ongoing in sugarcane for PRE weed control either on planted or ratoon cane. Sunflower, transplanted vegetables and perennial crops are also targets for future development of this herbicide. This herbicide has shown limited activity when applied POST.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Technical active ingredient is non-corrosive.
Storage stability: Technical active ingredient is not sensitive to oxidizing or reducing agents.
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent.
Emergency exposure: If contacted on skin, wash with plenty of soap and water. Get medical attention if irritation persists. If in eyes, flush with plenty of water. Call a physician if irritation persists. If inhaled, remove victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Susceptible plant species quickly exhibit necrotic symptoms and die within days of emergence.
Absorption/translocation: Oxadiargyl is active at germination as the new shoots come in contact with treated soil particles. Translocation following shoot uptake is very limited.
Metabolism in plants: NA
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: No resistant weed biotypes are known.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: NA
Other degradation: Oxadiargyl degraded fairly rapidly in four contrasting types of soils with a mean half-life of about 40 d. The two major metabolites of this herbicide are steadily degraded resulting in complete mineralization to carbon dioxide and a soil bound residue.
Persistence: Oxadiargyl dissipates rapidly from the water to the sediment phase and is readily degraded under anaerobic conditions.
Mobility: Oxadiargyl and its two major soil metabolites showed limited mobility in four contrasting soils and groundwater contamination is not expected.
Volatilization: NA
Formulation effects: Environmental fate properties are unaffected by formulation.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade oxadiargyl.
Acute toxicity:
Oral LD_{50} rat, > 5000 mg/kg; Dermal $LD_{50,}$ rabbit >2000 mg/kg; 4-h Inhalation LC_{50}, rat >5.16 mg/L; Primary eye irritation rabbit, non-irritating; Skin irritation rabbit, negative; Skin sensitization guinea pig, negative
Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA
Reproduction: NA
Mutagenicity:
Several unidentified tests showed that oxadiargyl technical was non-mutagenic (1).

Wildlife:

Bobwhite quail oral LD_{50}, >2000 mg/kg; 8-d dietary LC_{50}, >5200 mg/kg; NOEL, 5200 mg/kg; Daphnia 48-h EC_{50}, <0.37 mg/L; Bluegill sunfish 96-h LC_{50}, <0.37 mg/L; Rainbow trout 96-h LC_{50}, <0.37 mg/L

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Oxadiargyl was discovered by Rhone-Poulenc Agrochimie. It is currently under development in Asian-pacific countries.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Dickmann, R. et al. 1997. Proc. Brighton Crop Prot. Conf. Weeds, pp. 51-57.

oxadiazon

CAS #: 19666-30-9

14$^{(E)}$

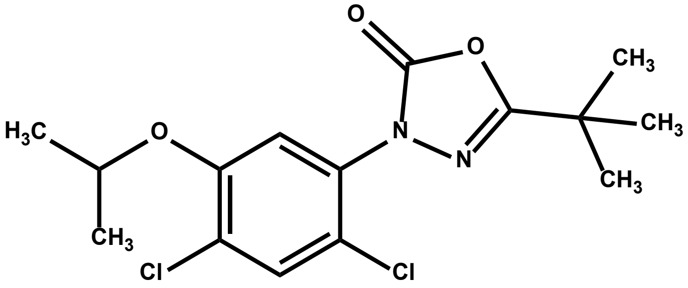
3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2-(3*H*)-one

NOMENCLATURE

Common name: oxadiazon (ANSI, BSI, ISO, JMAF, WSSA)
Other name(s): RP 17623; 5-*tert*-butyl-3-(2,4-dichloro-5-isopropoxyphenyl-1,3,4-oxadiazol-2(3*H*)-one (IUPAC)
Trade name(s): DELCUT®; PHARE®; RONSTAR®; RONSTAR® D FLO; RONSTAR® PL
Chemical family: oxadiazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
oxadiazon



Molecular formula: $C_{15}H_{18}Cl_2N_2O_3$
Molecular weight: 345.23 g/mole
Description: White crystalline powder, odorless
Density: 1.26 g/mL
Melting point: 87 C
Boiling point: NA
Vapor pressure: 1.03×10^{-4} Pa (25 C)
Stability: Stable to UV light; decomposed at ~230 C
Solubility:
water 0.7 mg/L (20 C)
organic solvents g/100 mL (20 C)
acetone ~60 ethanol ~10
isophorone ~60
methanol ~10
methylene chloride ~100
carbon tetrachloride ~60 methylethylketone ~60
chloroform ~100 toluene ~100
cyclohexane ~20
pK_a: None (non-ionizable)
K_{ow}: 63,100

HERBICIDAL USE

Oxadiazon can be soil-applied (before weed emergence) at 2.24-4.48 kg ai/ha on established or newly established bermudagrass, prerennial ryegrass, and fescue turf, and in various ornamentals. Oxadiazon controls many annual broadleaf and grass weeds including Florida pusley, *Oxalis* spp., stinging nettle, annual bluegrass, crabgrass spp., carpetweed, field sandbur, goosegrass, and green foxtail.

USE PRECAUTIONS

Fire hazard: Technical is non-flammable
Corrosiveness: Non-corrosive
Storage stability: Stable for >2yr
Cleaning glassware/spray equipment: Wash with detergent and rinse with water
Emergency exposure: Flush eyes with water for 15 min; get medical attention. No specific antidote is known; symptomatic treatment.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Seedlings emerge from treated soil but then wilt, followed by necrosis and desiccation. With foliar application, leaves of susceptible plants become chlorotic and then desiccated and necrotic within 1-2 d. Sublethal rates may produce foliar "bronzing", usually on young expanded leaves. Droplet drift may cause bleached spots or flecks on leaves.
Absorption/translocation: Soil-applied oxadiazon is readily absorbed by shoots of emerging seedling, but less so by roots. Foliar-applied oxadiazon is readily absorbed by leaves. It accumulates in older plant parts, with little movement to the growing points.
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:
K_{oc}: Average is 3200 mL/g (7). Strongly absorbed by soil colloids and organic matter.
Transformation: NA
Persistence: Moderate to long persistence with an average field half-life of 60 d (7)
Mobility: Low leaching potential due to strong adsorption to soil
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade oxidiazon unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >8000 mg/kg; LC_{50} rat, >194 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight
Subchronic toxicity: NA
Chronic toxicity:
24-mo dietary, rat: NOEL 10 mg/kg.d
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA

Wildlife:

Bobwhite quail oral LD_{50}, 6000 mg/kg; Mallard duck oral LD_{50}, >1000 mg/kg; Daphnia 48-h $LC_{50,}$ 0.5-8.0 mg/L; Carp 06-h LC_{50}, 1.76 mg/L; Catfish 96-h LC_{50}, ≥15.4 mg/L; Rainbow trout 96-h LC_{50}, 1->9 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Metabolites can be determined by GC with thermal-conductivity detection (2). Oxadiazon residues can be determined by GC with electrical conductivity detection (3) or by mass spectrometry (8). Residues in hops can be determined by GC (5).

Historical: First reported in 1969 (1). Introduced by Rhone-Poulenc Agrochimie, British patent 1,110,500 and U.S. patent 3,385,862.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Burgand, L. et al. 1969. 3rd Symp. New Herbic. P. 201.
2. Desmoras, J. et al. 1973. Anal. Meth. Pestic. Plant Growth Regul. 7:595.
3. Desmoras, J. et al. 1973. Anal. Meth. Pestic. Plant Growth Regul. 7:600.
4. Duke, S.O. et al. 1991. Weed Sci. 39:465.
5. George, D.A. 1982. J. Assoc. Off. Anal. Chem. 65:28.
6. Lee and Duke. 1994. Abstr. Weed Sci. Soc. Am. 34:52.
7. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
8. Yamamoto, Y. 1979. Biomed. Mass Spectrom. 6:2-5.

oxaziclomefone

CAS #: 153197-14-9

NC

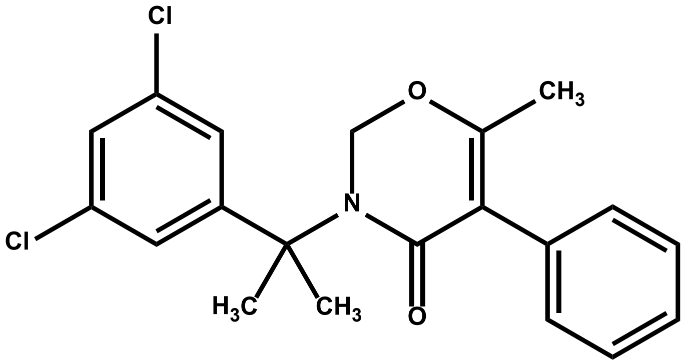
3-[1-(3,5-dichlorophenyl)-1-methylethyl]-2,3-dihydro-6-methyl-5-phenyl-4*H*-1,3-oxazin-4-one

NOMENCLATURE

Common name: oxaziclomefone (ISO accepted)
Other name(s): MY-100; 3-[1-(3,5-dichlorophenyl)-1-methylethyl]-3,4-dihydro-6-methyl-5-phenyl-2*H*-1,3-oxazin-4-one (IUPAC)
Trade name(s): NA
Chemical family: oxazinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
oxaziclomefone



Molecular formula: $C_{20}H_{19}Cl_2NO_2$
Molecular weight: 392.32 g/mole
Description: White crystals
Density: NA
Melting point: 149.5-150.5 C
Boiling point: NA
Vapor pressure: 1.33×10^{-5} Pa (50 C)
Stability: Stable
Solubility:
water 0.18 mg/L (20 C)
pK_a: NA
K_{ow}: 4.01

HERBICIDAL USE

Oxaziclomefone is used PRE or early POST at 30 to 80 g ai/ha in transplanted rice and at 25 to 50 g ai/ha in water seeded rice and provides effective control of *Echinochloa* spp., sedges and certain broadleaf weeds (1). Extensive field trials in Japan have shown that combinations of oxaziclomefone with sulfonylureas as a one-shot herbicide provide excellent selective control of both annual and perennial weeds when applied PRE or early POST in transplanted rice (1).

USE PRECAUTIONS

Fire hazard: Oxaziclomefone is not flammable
Corrosiveness: Product is non-corrosive
Storage stability: Technical active ingredient is not sensitive to oxidizing or reducing agents.
Cleaning glassware/spray equipment: Wash equipment and glassware with water and detergent.
Emergency exposure: If contacted on skin, wash with plenty of soap and water. Get medical attention if irritation persists. If in eyes, flush with plenty of water. Call a physician if irritation persists. If inhaled, remove victim to fresh air.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: The target site of oxaziclomefone has not yet been determined. It inhibits meristematic growth in a manner different than that of any other known herbicides. Biochemical investigations have shown partial reversal by gibberellic acid indicating cell wall biosynthesis as a likely target site. Further investigations are under way (1).
Symptomology: The initial symptoms of oxaziclomefone on *Echinochloa* spp. are observed in the new leaves, followed by chlorosis, reddish coloration of leaves and shoots (anthocyanin formation), necrosis and plant death. Under normal conditions, sensitive rice weeds are killed within 1-2 weeks of treatment, depending on their growth stage at application and also on weather conditions.
Absorption/translocation: Oxaziclomefone is applied POST in flooded rice paddies and thus it is absorbed by roots and shoots of treated plants.
Metabolism in plants: Not available; selectivity of oxaziclomefone to transplanted rice is mainly based upon physical selectivity rather than biological selectivity (1)
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: No resistant weed biotypes are known.

BEHAVIOR IN SOIL

Sorption: The soil sorption of oxaziclomefone in soil is very high.
Transformation:
Photodegradation: NA
Other degradation: Oxaziclomefone is hydrolyzed chemically in soils with half-lives ranging from 30 to 60 d at 50 C.
Persistence: Oxaziclomefone provided excellent control of *Echinochloa oryzicola* for 50 d after treaetment. The residual activity of oxaziclome at 60 g ai/ha was superior to mefenacet at 1200 g ai/ha under flooded conditions in the greenhouse. Oxaziclome has a very low risk of carryover to sensitive crops.
Mobility: NA
Volatilization: NA
Formulation effects: Environmental fate properties are unaffected by formulation type

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade oxaziclomefone

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, NA; Skin irritation rabbit, negative; Skin sensitization, guinea pig, negative

Subchronic toxicity:

Subchronic studies showed that all species tested tolerate high levels of oxaziclomefone for prolonged periods of time with few signs of toxicity.

Chronic toxicity:

Chronic studies showed that all species tested tolerate high levels of oxaziclomefone for prolonged periods of time with few signs of toxicity.

Teratogenicity:

Rat: Non-teratogenic
Rabbit: Non-teratogenic

Reproduction: NA

Mutagenicity:

Gene mutation: Ames mutagenicity test showed that oxaziclomefone technical is non-mutagenic.

Wildlife:

Oxaziclomefone technical: Carp, 48-h LC_{50} >5 mg/L

Use classification: Not yet assigned

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Oxaziclomefone was discovered in 1992 by Rhone-Poulenc Yuka Agro K.K. in Japan. It has been tested since 1993 and is currently under development in Asian-Pacific countries.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Jikihara, K. et al. 1997. Proc. Brighton Crop Prot. Conf. Weeds, pp. 73-80.

oxyfluorfen

CAS #: 42874-03-3

14$^{(E)}$

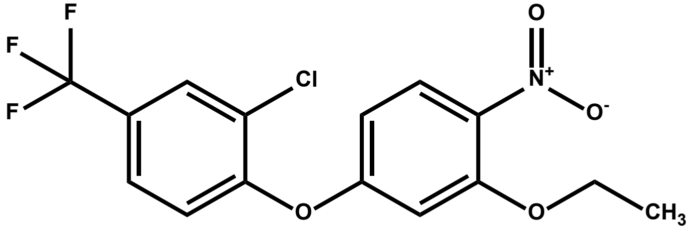
2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl) benzene

NOMENCLATURE

Common name: oxyfluorfen (ANSI, BSI, ISO, WSSA)
Other name(s):, oxyfluorfene (France); RH-2915; 2-chloro-α, α, α -trifluoro-*p*-toly-3-ethoxy-4-nitrophenyl ether (IUPAC)
Trade name(s): GALIGAN®; GOAL®; ORNA-MENTAL HERBICIDE II; ROUT®; KOLTAR, PINDAR GT
Chemical family: diphenylether; nitrodiphenylether; nitrophenylether

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
oxyfluorfen



Molecular formula: $C_{15}H_{11}ClF_3NO_4$
Molecular weight: 361.79 g/mole
Description: Semi-solid at room temperature, red-brown to yellow, faint smoky odor
Density: 1.35 g/mL (73 C)
Melting point: 76 - 80 C
Boiling point: 201.7 C
Vapor pressure: 2.67×10^{-4} Pa (25 C)
Stability: Decomposed by UV light; Decomposes at >240 C; No significant hydrolysis for 28 d at 25 C and pH 5,7, and 9
Solubility:
- water 0.1 mg/L (20 C)
- organic solvents g/100 mL (25 C)
- acetone 6
- isophorone 55.8
- *n*-butanol 13.8
- mesityl oxide 56.5
- chloroform 50-55
- methanol 16.7
- cyclohexane 11
- methylene chloride 58.5
- cyclohexanone 56.3
- methlisobutylketone 52.6
- dimethylformamide 62.5
- *n*-octanol 1
- *n*-hexane 3.4
- xylene 49.7

pK_a: None (non-ionizable)
K_{ow}: 29,400 (25 C)

HERBICIDAL USE

Oxyfluorfen can be applied as follows: PRE at 0.28-2.24 kg ai/ha in conifers, horseradish, taro, eucalyptus, and mint; before transplanting at 0.28-0.56 kg ai/ha in vegetable, fruit, nut, and vine crops and cottonwood; POST-directed at 0.56-2.24 kg ai/ha in artichokes (globe), citrus, corn, cotton, jojoba, papaya, taro, soybeans, fruit trees, nut trees, vines, and tropical plantation crops; and POST over-the-top ar 0.034-2.24 kg ai/ha in conifers, eucalyptus (pre bud break), cottonwood, clary sage, and onions. It also can be used at up to 0.56 kg ai/ha for fallow bed weed control before direct seedling of most vegetables, as well as cereals, cotton, and soybeans. Oxyfluorfen controls many annual small-seeded broadleaf weeds, such as filaree spp., *Malva* spp., fiddlenec, and groundsel, and suppresses annual grasses. It also controls topgrowth of nutsedge and johnsongrass when applied POST.

USE PRECAUTIONS

Fire hazard: GOAL 2XL and GOAL 1.6E are combustible but non-flammable; flash points are 99 C and 40 C, respectively.
Corrosiveness: Non-corrosive under normal conditions
Storage stability: GOAL EC formulations are stable for >2 yr, but temperatures ≤ 0 C may cause crystallization of the active ingredient.
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: Wash skin with soap and water; get medical attention if irritation persists. Flush eyes with water for at least 15 min; get medical attention. If ingested, do not induce vomiting; dilute by drinking 2 glasses of water.
Incompatibilities: Compatible with most other pesticides when used at normal rates. Avoid strong oxidizers.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Rapid leaf bleaching, desiccation, and necrosis, often localized around sites of spray droplet interception. General foliar necrosis follows with 1-2 d.
Absorption/translocation: Readily absorbed by leaves of most species, although low relative humidity may reduce absorption. Very little oxyfluorfen is absorbed by roots. Basipetal and acropetal translocation following root or shoot absorption is limited (3).
Metabolism in plants: Appears to be metabolized very slowly in plants.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Strongly absorbed to soil, and not readily desorbed (2). Desorption is irreversible in some soils. .
K_{oc} and K_d: Average K_{oc} is 100,000 mL/g (estimated) (5) K_{oc} 8076 mL/g and K_f 61.78 mL/g for absorption, and K_{oc} 11,518 mL/g and K_f 88.12 mL/g for desorption in a sandy

loam with 1.3% OM; K_{oc} 5585 mL/g and K_f 98.58 mL/g for adsorption, and K_{OC} 7103 mL/g and K_f 125.37 mL/g for desorption in a clay loam with 3.0% OM; K_{oc} 2891 mL/g and K_f 8.50 for adsorption, and K_{oc} 3211 mL/g and K_f 9.44 mL/g for desorption in a sand with 0.5% OM; K_{oc} 32,381 mL/g and K_f 228,61 mL/g for adsorption, and K_{oc} 4289 mL/g and K_f 30.28 mL/g for desorption in a silty loam with 1.2% OM.

Transformation:

Photodegradation: Half-life in water may be as short as 2/3 d, whereas the half-life on dry soil generally is 20-30 d. Photolysis is an important means of oxyfluorfen degradation in the environment.

Other degradation: Stable to hydrolysis over a wide range of soil pHs. Results indicate that microbial degradation rates are slow. In aerobic studies, detectable oxyfluorfen residues were CO_2 or were non-extractable (bound); half-life of extractable oxyfluorfen was 291-294 d in a clay loam and 556-596 d in a sandy loam. In anaerobic studies, no significant levels of metabolites were detected after 60 d in a sandy loam; half-life of extractable oxyfluorfen was estimated at 554-603 d.

Persistence: Moderate residual with an average field half-life of 30 d (5) that typically ranges from ~5-58 days

Mobility: Immobile on most soils, but slightly mobile on extremely sandy soils

Volatilization: Low losses, but may co-distill from moist soil surfaces

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade oxyfluorfen unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50} rat, 3.71 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, none; Eye irritation rabbit, none

GOAL 2XL: Oral LD_{50} rat, >2000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, 4.8 mg/L; Skin irritation rabbit, severe; Skin sensitization guinea pig, positive; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary mouse: NOEL <32 mg/kg/d (<200 ppm)

90-d dietary, rat: NOEL 144 mg/kg/d (1500 ppm)

90-d dietary, dog: NOEL 3 mg/kg/d (80 ppm)

28-d dermal, rat: NOEL 100 mg/kg/d

Chronic toxicity:

20-mo dietary, mouse: NOEL 0.3 mg/kg/d (2 ppm); non-statistically significant increase in incidence of liver tumors in males at the high dose (33 mg/kg/d; 200 ppm)

24-mo dietary, rat: NOEL 2 mg/kg/d (40 ppm); primarily liver effects; not carcinogenic

24-mo dietary, dog: NOEL 3 mg/kg/d (100 ppm); liver effects

Teratogenicity:

Rat: Maternal NOAEL >1000 mg/kg/d; Developmental NOAEL >1000 mg/kg/d. No evidence of developmental effects.

Rabbit: Maternal NOAEL 30 mg/kg/d; Developmental NOAEL 30 mg/kg/d. Increased late resorptions, decreased live fetuses/doe at maternally toxic dose levels of 90 mg/kg/d..

Reproduction:

Rat: Parental NOAEL 31/33 mg/kg/d (M/F; 400 ppm); Offspring NOAEL 31/33 mg/kg/d (M/F; 400 ppm) based on decreased BW/smaller litter size at maternally toxic dose levels of 120/131 mg/kg/d (M/F; 1600 ppm)

Genetic toxicity:

Newer technical material (96-98% purity) was tested in 12 genetic toxicology studies. All assays were negative except for one Ames mutagenicity assay which was positive only at high, insoluble levels. A subsequent Ames assay with 96% purity test material was negative.

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg body weight; 8-d dietary $LC_{50,}$ >5000 mg/kg diet; reproduction NOEL, 750 mg/kg diet; Mallard duck, 8-d dietary LC_{50}, >5000 mg/kg diet; reproduction NOEL, 500 mg/kg diet; Honey bee oral LC_{50}, >100 ug/bee; Daphnia, 48-h LC_{50}, >1 mg/L, reproduction MAC >0.13 <0.028 mg/L; Bluegill sunfish 96-h LC_{50} 0.2 mg/L; Channel catfish 96-h LC_{50} 0.4 mg/L; Minnow reproduction MAC >0.038<0.074 mg/L; Rainbow trout 96-h LC_{50} 0.4 mg/L; Eastern oyster LC_{50}, 0.0693 mg/L; Fiddler crab LC_{50}, >1000 mg/L; Freshwater clam LC_{50}, 10 mg/L; Grass shrimp LC_{50}, 0.032 mg/L; Green algae 96-h EC50, 0.00029 mg/L; Duckweed 14-d EC50 = 0.00032 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React 3,4-dichlorobenzotrifluoride and resorcinol. The resulting intermediate is nitrated and then ethoxylated to produce oxyfluorfen.

Analytical methods: Available from DowAgro Sciences

Historical: First reported in 1975 (6). Introduced by Rohm and Haas Company; U.S. patent 3,798,276. First registration occurred in 1976, although first U.S. registration was in 1979.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry Source(s): Adama, Dow AgroSciences

Reference(s):

1. Duke, S.O. et al. 1991. Weed Sci. 39:465.
2. Fadauomi and Warren. 1977. Weed Sci. 25:97.
3. Fadayomi and Warren. 1977. Weed Sci. 25:111.
4. Lee and Duke. 1994. Abstr. Weed Sci. Soc. Am. 34:52.
5. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1
6. Yih and Swithenbank. 1975. J. Agric. Food Chem. 23:592.

paraquat

1,1′-dimethyl-4,4′-bipyridinium ion

CAS# Cation: 4685-14-7
Dichloride salt: 1910-42-5

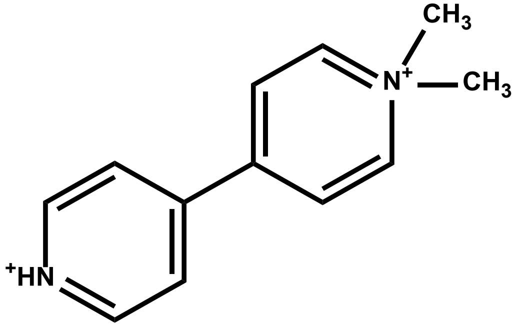
22$^{(D)}$

NOMENCLATURE

Common name: paraquat (ANSI, BSI, ISO, WSSA)
Other name(s): methyl viologen; PP 148; 1,1′-dimethyl-4,4′-bipyridinium (IUPAC)
Trade name(s): GRAMOXONE®; BOA®; CEKUQUAT; CYCLONE®; DEXTRONE; DEXTRONEX; DEXURON; ESGRAM; FIRESTORM™; GOLDQUAT 276; GRAMOXONE® SUPER TRES; HERBAXON; HERBAXONE; PARAZONE™ 3SLPAQUAT; PILLARQUAT; PILLARXONE; STARFIRE®;SWEEP; TOXER; WEEDOL
Chemical family: bipyridilium; bipyridinium; dipyridilium; quaternary ammonium

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
paraquat cation



Molecular formula: *Cation* $C_{12}H_{14}N_2$; *Dichloride salt* $C_{12}H_{14}Cl_2N_2$
Molecular weight: *Cation* 186.26 g/mole; *Dichloride salt* 257.16 g/mole
Description: White crystalline solid
Density: 1.5 g/mL (25 C)
Melting point: 340 C
Boiling point: NA
Vapor pressure: 1 x 10^{-4} Pa
Stability: Degraded by UV light; decomposes at ~300 C; unstable in alkaline solution.

Solubility:
water 620,000 mg/L (25 C)(8)
organic solvents (25 C):
acetone slightly soluble
hydrocarbons insoluble
carbon disulfide insoluble
kerosene insoluble
ethanol insoluble
dimethylformamide slightly soluble

pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = -4.5 (20 C)

HERBICIDAL USE

Paraquat is a non-selective, foliar-applied herbicide, often used to control existing vegetation at planting in no-till. It can be applied preplant or PRE in many agronomic crops, vegetables, flowers, and fruits at rates ranging from 0.28-1.05 kg cation/ha. Other uses include: dormant season in established alfalfa, clover, mint, and rhubarb; between cuttings at 0.28 kg cation/ha in established alfalfa; pre-harvest at 0.34-0.53 kg cation/ha in drybeans, sunflowers, guar, potatoes, and soybeans; POST-directed at 0.53 kg cation/ha in corn, sorghum, soybeans, sugarcane, pineapple, small fruits, cassavas, taniers, yams, pigeon peas, strawberries, trees and vines, guava, hops, tomatoes, and peppers; weed control in fallow (including Conservation Reserve and Federal Set-aside programs) and non-cropland; and pre-harvest desiccation of potato vines and weed control in rubber and coffee plantations. A non-ionic surfactant or oil adjuvant is required for maximum efficacy.

USE PRECAUTIONS

Fire hazard: All products are aqueous and non-combustible. However, paraquat and aluminum react to produce hydrogen gas which may form a highly combustible gas mixture which could explode if ignited.
Corrosiveness: Paraquat corrodes aluminum (see Fire Hazard), and in concentrated form may be slightly corrosive to certain other metals. Dilute spray-tank solutions generally are non-corrosive to most materials used in spray equipment.
Storage stability: Shelf life is indefinite under normal storage conditions. Dry technical paraquat is somewhat sensitive to UV light. All products are stable to heat beyond the range of ordinary room temperature. Store above 0 C.
Cleaning glassware/spray equipment: Flush equipment with water.
Emergency exposure: If ingested, immediately induce vomiting. Administer fluids and induce further vomiting. Seek immediate medical attention. Paraquat can be lethal if ingested in small amounts and treatment must begin immediately.
Incompatibilities: Not compatible with some alkyl sulfonate or alkyl aryl sulfonate wetting agents or alkali-metal salts of hormone weed killers; can hydrolyze in alkaline solution.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem I (PS I) (more details on page 15)
Symptomology: Rapid wilting and desiccation beginning within several h of application in full sunlight. Complete foliar necrosis occurs in 1-3 d.
Absorption/translocation: Rapidly absorbed into foliage and is rainfast 30 min after application. Rapid foliar uptake requires a non-ionic surfactant. More than 50% of applied paraquat was absorbed by leaf tissues of three species within 1 h (2). Paraquat translocates only in the apoplast (including the xylem), and thus foliar-applied paraquat

remains in treated leaves under normal conditions. When soil moisture is low and relative humidity high, paraquat residues in desiccating potato vines may move to the tubers in response to basipetal xylem flow facilitated by water demands of the growing tubers.

Metabolism in plants: Paraquat apparently is not metabolized in higher plants. Paraquat remaining on the plant surface, however, is photodegraded about 25-50% in 3 wk of bright sunlight, producing *N*-methyl isonicotinic acid which later degrades to methylamine (6). Since plants are killed rapidly in bright sunlight, significant quantities of the breakdown products are formed only on the surface of dead tissues.

Non-herbicidal biological properties: Paraquat is highly toxic in mammalian systems. No insecticidal or nematocidal properties are known, although it can be used to control columnaris, a myxobacterial disease of fish.

Mechanism of resistance in weeds: Paraquat resistance has been confirmed in at least 12 species. The mechanism(s) of resistance is controversial and may be due to elevated activities of enzymes that protect against toxic effects of oxygen radicals (7) or to sequestration or exclusion of the herbicide from the target site (5).

BEHAVIOR IN SOIL

Sorption: Rapidly and tightly adsorbed to soil, primarily to clay particles. The dicationic paraquat forms ionic bonds with negatively charged clays, even inserting into the layer planes of montmorillonite clay. Paraquat is completely inactive in soil.

K_{oc}: Estimated at 1,000,000 mL/g (8)

Transformation:

Photodegradation: Can be degraded from desiccated plant surfaces and possibly from soil surfaces to the extent of 25-50% in 3 wk under bright sunlight.

Persistence: Highly persistent with an average field half-life estimated at 1000 d (8). However, paraquat residues are tightly adsorbed and biologically unavailable in soil.

Mobility: Completely immobile in soil due to extremely tight adsorption. No leaching potential.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade paraquat dichloride salt unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 112-150 mg/kg; monkey, 50 mg/kg; cat, 48 mg/kg; cow, 50-75 mg/kg; Dermal LD_{50} rabbit, 240 mg/kg; 4-h inhalation LC_{50} rat, nontoxic; Skin irritation rabbit, yes; Skin sensitization guinea pig, no; Eye irritation, NA.

GRAMOXONE EXTRA: Oral LD_{50} rat, 40-150 mg/kg; Dermal LD_{50} rabbit, 240 mg/kg; Skin irritation rabbit, mild; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe. **CYCLONE:** Oral LD_{50} rat, 40-150 mg/kg; Dermal LD_{50} rabbit, 240 mg/kg; Skin irritation rabbit, mild (repeated exposure can cause skin damage, edema, and ulcerations); Skin sensitization guinea pig, yes; Eye irritation rabbit, severe.

Subchronic toxicity: NA

Chronic toxicity:

24-mo dietary, rat: NOEL 25 mg/kg; not carcinogenic

24-mo dietary, dog: NOEL 34 mg/kg/d

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail oral LD_{50}, 981 mg/kg; Japanese quail oral LD_{50}, 970 mg/kg; Mallard duck oral LD_{50}, 4048 mg/kg; Rhode Island hen oral LD_{50}, 262 mg/kg; Brown trout 96-h LC_{50}, 2.5-13 mg/L; Rainbow trout 96-h LC_{50}, 32 mg/L

Use classification: Restricted use because of high mammalian toxicity

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Direct quaternization of 4,4′-bipyridyl with chloromethane under pressure with or without solvent. The iodide salt may be exchanged with the chloride salt or methylsulfate ion by use of ion exchange. Silver methylsulfate gives a quantitative exchange for the halide form.

Purification of technical: Paraquat dichloride may be isolated from the formulated product by adding gradually (with rapid stirring) 1 volume of paraquat formulation to 10-15 volumes of a 1:1 mixture of acetone:isopropanol. Filter and rinse the solid with acetone:isopropanol. Purify by dissolving the solid in a minimum amount of water and repeating the precipitation.

Analytical methods: Methods for formulated product analysis and residue analysis are available (Pages 475-481 *in* G. Zweig, ed. 1967. Analytical Methods for Pesticides, Plant Growth Regulators and Food Additives, Vol. V. Academic Press, New York). Both methods are based on spectrophotometric measurement.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama, Chemtura; Griffin; Syngenta Crop Protection

Reference(s):

1. Brian, R. C. 1958. Nature (London) 181:446
2. Brian, R. C. 1967. Ann. Appl. Biol. 59:91.
3. Calderbank, A. 1968. Adv. Pest Control Res. 8:127.
4. Dodge, A. D. 1982. Pages 57-77 *in* D. E. Moreland, J. B. St. John, and F. D. Hess, eds., Biochemical Responses Induced by Herbicides. Am. Chem. Soc. Symp. Ser. No. 181, Washington D.C.
5. Fuerst and Vaughn. 1990. Weed Technol. 4:150.
6. Funderburk and Lawrence. 1964. Weeds 12:259.
7. Shaaltiel and Gressel. 1986. Pestic. Biochem. Physiol. 26:22.
8. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

pebulate

S-propyl butylethylcarbamothioate

CAS #: 1114-71-2

8(N)

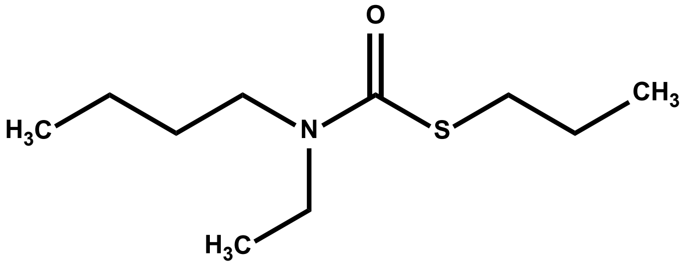
NOMENCLATURE

Common name: pebulate (BSI, ISO, WSSA)
Other name(s): R-2061; *S*-propyl butyl(ethyl) thiocarbamate (IUPAC)
Trade name(s): TILLAM®; EDGE®; PEBC
Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

Pebulate



Molecular formula: $C_{10}H_{21}NOS$
Molecular weight: 203.34 g/mole
Description: Yellow liquid, amine-like odor
Density: 0.96 g/mL (20 C)
Melting point: NA (liquid at room temperature)
Boiling point: 142 C (2.80 x 10^3 Pa)
Vapor pressure: 1.19 Pa (25 C)
Stability: Stable at 54.5 C for 6 wk, and at room temperature for 2 yr; reacts with oxidizing but not with reducing agents.
Solubility:

water 60 mg/L (20 C)
organic solvents (25 C):
miscible in acetone, ethanol, kerosene, methylisobutyl ketone, 4-methylpentan-2-one, xylene

pK_a: None (non-ionizable)
K_{ow}: 9600 (25 C)

HERBICIDAL USE

Pebulate can be applied as follows: PPI or through subsurface sweeps at 1.12 or 4.5 kg ai/ha in tobacco; PPI at 3.4-6.7 kg ai/ha in sugarbeets; and PPI, layby incorporated, or through solid set sprinkler irrigation systems at 4.5-6.7 kg ai/ha in tomatoes. It must be applied soon after application to prevent volatilization losses. Pebulate can be applied by conventional sprayer in water or liquid fertilizer, or impregnated on dry bulk fertilizer. Pebulate primarily controls annual grasses, including barnyardgrass, crabgrass spp., foxtail spp., goosegrass, and wild oats. It also controls yellow and purple nutsedge along with certain annual broadleaf weeds.

USE PRECAUTIONS

Fire hazard: TILLAM is non-flammable; flash point (TOC) is 124 C; fire point is 132 C.
Corrosiveness: Non-corrosive
Storage stability: Apparently indefinite storage life under ambient conditions.
Cleaning glassware/spray equipment: Wash glassware with solvent followed by water; flush equipment with water.
Emergency exposure: Flush skin with water; get medical attention. Flush eyes with water for at least 15 min; get medical attention if irritation occurs. If ingested, drink several glasses of water, but do not induce vomiting; consult a physician.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)
Symptomology: Most susceptible plants fail to emerge. Germination is not inhibited but growth of grass coleoptiles or broadleaf epicotyls ceases below the soil surface.
Absorption/translocation: Readily absorbed by the shoot and root systems of emerging seedlings. Pebulate also is absorbed by roots of established plants and translocated throughout stems and leaves via the apoplast.
Metabolism in plants: CO_2 evolution resulting from hydrolysis and decarboxylation reactions on the alkyl or carbonyl groups of pebulate was detected in mung beans, wheat, corn, and peas (3, 4). Pebulate may be oxidized to pebulate-sulfoxide (7).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

.

BEHAVIOR IN SOIL

Sorption: Adsorbed onto dry soil

K_{oc}: Average is 430 mL/g (8)

Transformation: Primarily degraded by microbes
Persistence: Short persistence with a half-life of ~2 wk in moist loam soil at 21-27 C. Pebulate residues do not persist long enough to injure susceptible crops planted 1 yr after application.
Mobility: Leaches fairly readily. Pebulate leaches more than EPTC, but less than cycloate.
Volatilization: Readily lost from wet soil surfaces when not incorporated immediately after application.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pebulate unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 1675 mg/kg, male mouse, 1652 (1529-1784) mg/kg; Dermal LD_{50} rabbit, 4640 mg/kg; 4-h inhalation LC_{50}, 0.0036 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

TILLAM 6-E: Oral LD_{50} male rat, 1400 mg/kg, female rat, 1390 mg/kg; Dermal LD_{50} rabbit, 2000 mg/kg; Skin irritation rabbit, severe; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL 16 mg/kg/d

90-d dietary, dog: NOEL 20 mg/kg/d

Chronic toxicity:

12-mo dietary, dog: NOEL 5 mg/kg/d.

Teratogenicity: NA

Reproduction: NA

Mutagenicity: NA

Wildlife:

Bobwhite quail oral LD_{50}, 8400 mg/kg, 7-d dietary LC_{50}, 8400 mg/kg; Mallard duck, oral LD_{50}, >2000 mg/kg, 8-d dietary LC_{50}, >10,000 mg/kg; Honey bee oral LD_{50}, 11 µg/bee; Daphnia 48-h LC_{50}, 2.1; Bluegill sunfish 96-h LC_{50}, 7.4 mg/L; Rainbow trout 96-h LC_{50}, 7.4 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React *n*-propyl chlorothiolformate with *n*-butyl ethyl amine and base.

Purification of technical: NA

Analytical methods: Pebulate can be separated from impurities on several columns and detected by GC with either thermal conductivity or flame ionization detectors.

Historical: First reported in 1959 (1). Introduced by Stauffer Chemical Co. (now Syngenta); U.S. patent 3,175,897.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Burt, E. O. 1959. Proc. 12th South. Weed Control Conf. p. 19.
2. Casida, J. E. et al. 1974. Science 184:573.
3. Fang and George. 1962. Plant Physiol. 37S:26.
4. Fang, S. C. 1975. Pages 323-348 *in* P. C. Kearney and D. D. Kaufman, eds., Herbicides: Chemistry, Degradation, and Mode of Action. Marcel Dekker, Inc., New York.
5. Fuerst, E. P. 1987. Weed Technol. 1:270.
6. Gronwald, J. W. 1991. Weed Sci. 39:435.
7. Hubbel and Casida. 1977. J. Agric. Food Chem. 25:404.
8. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

pelargonic acid

CAS #: 112-05-0 **26**$^{(Z)}$

nonanoic acid

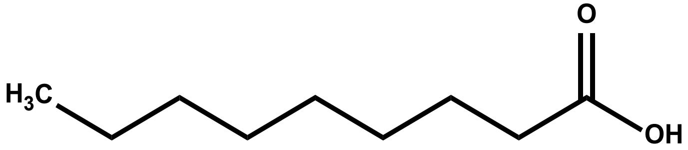
NOMENCLATURE

Common name: pelargonic acid (IUPAC, WSSA)
Other name(s): NA
Trade name(s): SCYTHE
Chemical family: carboxylic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

pelargonic acid



Molecular formula: $C_9H_{18}O_2$
Molecular weight: 158.24 g/mole
Description: Water-white liquid; a waxy fatty acid like odor similar to crayons
Density: 0.904 g/mL (25 C)
Melting point: 12.5 C (technical)
Boiling point: 230-237 C at atmospheric pressure
Vapor pressure: 2.67 x 10^3 Pa (253 C)
Stability: Typical of straight chain carboxylic acid chemistry
Solubility: Very slightly soluble in water and readily soluble in most organic solvents.
pK_a: NA
K_{ow}: NA

HERBICIDAL USE

SCYTHE is a contact, non-selective, broad spectrum, foliar-applied herbicide. It only controls actively growing emerged green vegetation. It provides burndown of both annual and perennial broadleaf and grass weeds, as well as most mosses and other cryptogams. The degree of burndown and the longevity of control is less when plants are inactive, mature, or biennial/perennials. This product does not translocate and it will burn only those plant parts that are coated with spray solution. Visible effects occur within hours. Repeat treatments are necessary for new plants emerging from seed or regrowth of treated vegetation. SCYTHE may be used for vegetative burndown in many situations. As a stand-alone treatment or mixture with residual herbicides, rates of 3-7% (v/v) solution provide varying degrees of burndown. For tank mixtures with foliar herbicides, rates lower than 3% (v/v) should be used. Synergistic responses with certain POST herbicides show enhanced speed of top kill and improved control of numerous weed species. The compound is protected under U.S. patent 5,196,044.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable. The flash point for pelargonic acid is 140 C by Pensky Martin closed cup. The fire point is 146 C.
Corrosiveness: Pelargonic acid is mildly reactive with some metals. The acid is typically shipped in aluminum tankers or lined drums. Corrosiveness is not a problem with spray solutions.
Storage stability: Shelf-life is very long. Freeze point of pure pelargonic acid is < 12.5 C. SCYTHE freezes at -4 C. Frozen material quickly returns to the liquid state without segregation of components.
Cleaning glassware/spray equipment: Triple rinse with water.
Emergency exposure: Protective eyeware and gloves are recommended. Removal from skin can be accomplished by washing with soap and water. If eye contact occurs, flush immediately with water and get further medical attention.
Incompatibilities: The formulated concentrate is an emulsifiable product. Care should be taken to avoid tank mixing products that could destabilize the emulsion, such as liquid fertilizers and other strongly ionic materials.

BEHAVIOR IN PLANTS

Mechanism of action: Pelargonic acid causes rapid cell death. Bleaching of chloroplasts and general ion leakage are apparent within minutes of treatment. The mechanism of action is not completely defined; however, it appears that the primary effect of the chemical is to affect a sudden decrease in intracellular pH which in turn causes loss of membrane integrity and ultimately cell death.
Symptomology: The symptoms are typical of rapid burndown activity. Within minutes after application, the treated foliage begins to darken and takes on a water-soaked appearance. This is followed by general wilting desiccation, and death of the treated tissue. Depending upon temperature, this process is complete in one to several hours.
Absorption/translocation: Pelargonic acid is absorbed into green tissue through the cuticle, but it does not move systematically in the plant or penetrate woody tissue. All effects are restricted to the site of original contact. Pelargonic acid has been demonstrated to synergize the activity of several
Metabolism in plants: Hypothetically, pelargonic acid is deprotonated as it enters the cell. It may later be metabolized through the normal beta-oxidation of fats, but this is not related to its herbicidal activity.
Non-herbicidal biological properties: The active ingredient has potent insecticidal and fungicidal activity. However, its practical use against those targets is limited by its phytotoxicity. Pelargonic acid can be used for contact control of moss, lichens, certain algae, and other cryptogams.
Mechanism of resistance in weeds: There are no known

cases of resistance. Plants differ in their sensitivity to the herbicide primarily in terms of their cuticular resistance to uptake.

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Persistence: Non-persistent in soil
Mobility: NA
Volatilization: Relatively volatile, but the vapors do not damage plants.
Formulation effects: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pelargonic acid unless specified otherwise.

Acute toxicity:

Oral LD_{50} rat, > 5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, >1244 mg/L; Primary eye irritation rabbit, severe; Skin irritation rabbit, severe; Skin sensitization guinea pig, none

SCYTHE Formulation: Oral LD_{50} rat, > 5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.29 mg/L; Primary eye irritation rabbit, severe; Skin irritation rabbit, moderate; Skin sensitization guinea pig, none

Subchronic toxicity:

90-d dietary, rat: NOEL >1834 mg/kg/d (> 20,000 mg/kg)

Chronic toxicity:

18-mo dietary, mouse: NOEL >50 mg/kg/d; not oncogenic

Teratogenicity:

Rat: NOEL >1000 mg/kg/d. Not teratogenic

Reproduction: NA

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

DNA damage/repair: Chromosomal aberration assay, negative; Cytogenic assay, negative

Other tests: Mouse Lymphoma Forward Mutation Assay, negative without metabolic activation; positive in the presence of metabolic activation; *In vivo* mouse micronucleus, negative; *Salmonella* mammalian microsome reverse mutation assay, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Honey bee 48-h acute LD_{50}, >25 mg/bee; Daphnia 48-h EC_{50}, >96 mg/L; Bluegill sunfish 96-h acute LC_{50}, >295 mg/L; Rainbow trout 96-h LC_{50}, >91 mg/L

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Pelargonic acid is a naturally occurring fatty acid which can be found at appreciable concentrations in a variety of plant and animal products. Its practical commercial production is based on ozonolysis of oleic acid at about 90% purity. It can also be produced synthetically.
Purification of technical: NA
Analytical methods: Gas chromatography procedures are available upon request from Dow AgroSciences.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Gowan.
Reference(s):

1. Berrie, A.A.M. et al. 1975. Plant Sci. Lett. 6: 163.
2. Caulder, J. et al. 1993. Process and composition for controlling weeds. United States Patent #5,196,044.
3. Crowley, R.H., et al. 1991. Proc. South. Weed Sci. Soc. 43: 207.
4. Ha, J. Kim and R.C. Lindsay. 1991. JAOCS. 68: 294.
5. Puritch, G.S. 1991. United States Patent # 5,035,741.

pendimethalin

CAS #: 40487-42-1 $3^{(K_1)}$

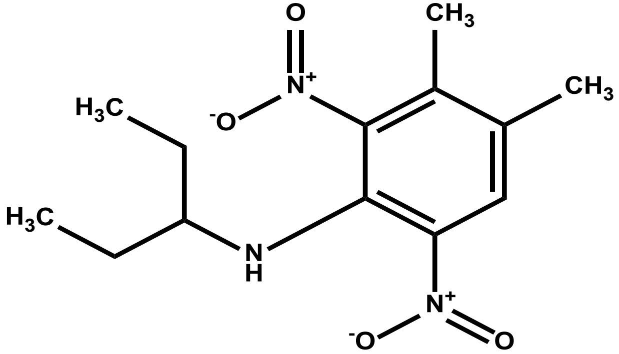
N-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitrobenzenamine

NOMENCLATURE

Common name: pendimethalin (ANSI, BSI, ISO, WSSA)
Other name(s): AC 92,553; CL 92,553; pendimethaline; penoxalin (discontinued common name); *N*-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine (IUPAC); *N*-(1-ethylpropyl)-3,4-dimethyl-2,6-dinitroaniline
Trade name(s): HELENA® PENDIMETHALIN; PENDULUM®; PENDULUM AQUACAP™; PROWL®; PROWL® H_2O; PURSUIT® PLUS; ACUMEN®; FRAMEWORK®; FREEHAND®; STEALTH®
Chemical family: dinitroaniline

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
pendimethalin



Molecular formula: $C_{13}H_{19}N_3O_4$
Molecular weight: 281.31 g/mole
Description: Crystalline orange-yellow solid with faint nutty odor
Density: 1.17 g/mL (25 C)
Melting point: 47-57 C
Boiling point: 330 C (estimated)
Vapor pressure: 1.25×10^{-3} Pa (25 C)
Stability: Stable in acid and base; Decomposes at ~200 C; slowly decomposed by UV light
Solubility:
water 0.275 mg/L (25 C)
organic solvents g/1000 mL (25 C)
acetone 161
DMSO 21.4
n-heptane 11.2
methanol 5.5
methylene chloride 232
toluene 128.4
xylene soluble
pK_a: None (non-ionizable)
K_{ow}: 152,000

HERBICIDAL USE

Pendimethalin can be applied as follows: PRE or early POST at 0.84-2.24 kg ai/ha in field and sweet corn; POST at 0.84-1.12 kg ai/ha in grain sorghum and rice; PPI or PRE at 0.56-1.68 kg ai/ha in soybeans and cotton; POST at 0.84-1.68 kg ai/ha in wheat; PRE, PRE incorporated, or early POST at 0.84-1.68 kg ai/ha in potatoes; PPI or at layby at 0.84-1.68 kg ai/ha in tobacco; PPI at 0.56-1.12 kg ai/ha in peanuts; PRE through layby at 2.24-3.36 kg ai/ha in sugarcane; PPI at 0.56-1.68 kg ai/ha in sunflowers and beans (dry, lima, snap, chickpeas, and Southern peas); PRE at 0.56-1.68 kg ai/ha in sweet lupines; PRE or POST at 0.84-1.68 kg ai/ha in garlic; PPI or PRE at 0.56-1.4 kg ai/ha in forage legumes; PRE (muck soil only) or early POST in direct-seeded or transplanted dry bulb onions or shallots; and PRE in fruit and nut crops and vineyards. Other labeled crops and uses for pendimethalin include alfalfa, certain perennial grasses grown for seed production and perennial warm-season grasses, selected vegetables, clover for seed production, fallow, lentils, mint, and strawberry. Pendimethalin can also be used as a preemergence weed control herbicide in ornamental production, landscape and grounds maintenance, turfgrass, and other specified noncrop areas. Pendimethalin controls primarily grass weeds, including barnyardgrass, crabgrass spp., *Panicum* spp., foxtail spp., goosegrass, seedling johnsongrass, signalgrass, and shattercane, with control of certain broadleaf weeds such as lambsquarters, redroot pigweed, and velvetleaf. For certain crops, pendimethalin can be applied in liquid fertilizer, impregnated on dry bulk fertilizer, or applied through chemigation systems.

USE PRECAUTIONS

Fire hazard: Pendimethalin technical and PROWL 3.3 EC are non-flammable; flash points are >97 C.
Corrosiveness: Non-corrosive
Storage stability: Pendimethalin is stable, PROWL 3.3 EC should not be stored at <4.4 C or >49 C
Cleaning glassware/spray equipment: Detergent wash for technical and formulated products; pre-rinsing glassware with organic solvent may be needed for technical; yellow staining of plastics and fiberglass should be expected.
Emergency exposure: If PROWL 3.3 EC is ingested, do not induce vomiting. Due to increased risk of chemical pneumonia or pulmonary edema caused by aspiration of hydrocarbons into the lungs, vomiting should only be induced under professional supervision. If PROWL 3.3 EC contacts eyes, flush with water. If PROWL 3.3 EC contacts skin, wash with soap and water. Get medical attention if irritation persists.
Incompatibilities: PROWL 3.3 EC should be mixed in the spray tank before adding LEXONE® DR with spray volumes of 47-93 L/ha. PROWL 3.3 EC should be mixed with SENCOR® DR only with spray volumes of >93 L/ha, and mixed with BICEP® 6L at spray volumes of 47-93 L/ha only if PROWL 3.3 EC is added to the spray tank first. If spray water pH is ≥7.5, if water hardness is high, or when the carrier is liquid fertilizer, PROWL 3.3 EC should be added to the spray tank before addition of ZORIAL® DF. When carrier water is alkaline, the addition of a buffering agent before mixing of ZORIAL DF may be beneficial. PROWL 3.3 EC

should be mixed in the spray tank before adding EVIK® 80W and with carrier volume >187 L/ha. Addition of a compatibility agent adding PROWL but before adding EVIK may improve compatibility.

BEHAVIOR IN PLANTS

Mechanism of action: Mitotic disruption through inhibition of the microtubule protein tubulin (more details on page 12)

Symptomology: Highly susceptible annual grasses and broadleaves usually fail to emerge. Coleoptile growth in grasses is inhibited. Emerged grass shoots are deformed. Stems of broadleaves can become brittle at the soil line. Broadleaf hypocotyls may also swell at and just above the soil line. The most easily-recognized symptom is root growth inhibition, especially in lateral (secondary) roots. Roots tips become thickened and stubby (typically called clubbed roots).

Absorption/translocation: Pendimethalin is soil-applied and is absorbed by roots and coleoptiles. The most important absorption site for highly sensitive grasses appears to be the coleoptile. Translocation is not important in controlling unemerged weed seedlings because absorption occurs in the coleoptile and roots where herbicidal action takes place. Pendimethalin is highly lipophilic and should rapidly partition into membranes and other lipid components of root tissue. Thus, acropetal translocation is emerged plants is small.

Metabolism in plants: Pendimethalin is oxidized at the 4-methyl group on the benezene ring and the *N*-1-ethylpropyl group in the amine moiety.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Trifluralin-resistant goosegrass from the southern U.S. is also resistant to other dinitroaniline herbicides, including pendimethalin (2). The resistance mechanism may involve either a change in the binding site on tubulin subunits (5) or an altered microtubule-associated protein (6). Populations of slender foxtail (*Alopecurus myosuroides*) from England are resistant to pendimethalin, but not to other dinitroanilines (1). These populations are cross-resistant to diclofop and chlortoluron, and resistance may be due to faster detoxification by oxidation of the ring methyl group (1).

BEHAVIOR IN SOIL

Sorption: Strongly absorbed by clay and OM

K_{oc} K_f and 1/n: Average K_{oc} is 17,200 mL/g. K_{oc} 15,000 mL/g, K_f 30, and 1/n 0.95 for a loamy sand with 3.2% clay, 0.8% OM, and pH 5.8; K_{oc} 13,000 mL/g, K_f 110 mL/g, and 1/n 0.92 for a sandy loam with 11.2% clay, 1.6% OM, and pH 6.4; K_{oc} 14,100 mL/g, K_f 380 mL/g, and 1/n 1.13 for a silt loam with 19.2% clay, 4.7% OM, and pH 7; 13,700 mL/g, K_f 301 mL/g, and 1/n 0.83 for a loam with 15% clay, 3.8% OM, and pH 7; K_{oc} 29,400 mL/g, K_f 854 mL/g, and 1/n 1.21 for a silty clay loam with 25% clay, 5% OM, and pH 6.5

***K_d*:** K_f values describe pendimethalin adsorption better than K_d values.

Transformation:

Photodegradation: Half-life is 7 d in water (25 C) in full summer sunlight. Absorption maximum in water is 290 nm. Less than 5% degraded by 30 d after application on a sandy loam with 11% clay, 1.6% OM, pH 6.4 and held at 10.2% moisture. Contribution to field dissipation is minor

Other degradation: Rapid degradation under anaerobic conditions. Aerobic biological degradation is slow.

Persistence: Typical half-life in the field is 44 d, but varies with soil temperature and moisture. Incorporation slows pendimethalin dissipation.

Lab experiments: Half-life at 30 C and 75% field capacity (FC): sandy loam 45 d, clay loam 54 d clay 42 d; half-life in a clay loam at 75% FC: 101 d at 10 C, 77 d (20 C), 61 d (35 C); half-life in clay loam (30 C): 73 d (50% FC), 56 d (100% FC) (7).

Mobility: Pendimethalin is immobile, being strongly bound to OM and clay. Little solubilized pendimethalin residues are available for runoff due to strong binding to soil, especially where incorporated. Most pendimethalin washed into surface water via sediment would remain bound to sediment and unavailable to aquatic organisms.

Volatilization: Pendimethalin is moderately volatile. Slight losses can occur with high temperature, moist soil, and wind. Mechanical incorporation or activation by rainfall within 7 d after application prevent appreciable losses.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: U.S. patents 24, 885, 25,658, and others

Purification of technical: NA

Analytical methods: Pendimethalin and its 4-(hydroxyl methyl) metabolite are extracted from foliage with aqueous acid/methanol, from seeds and meal with chloroform/methanol, and from oil with hexane. After removal of many coextractive by solvent partitionings, final clean-up is achieved on florisil. Residues are detected using GC with an electron capture detector versus an external standard. Validated sensitivity is 50 mg/kg.

Historical: Pendimethalin was discovered in 1971 by American Cyanamid; Belgium patent 816,837 and U.S. patent 4,199,669. First reported in 1974 (3). It was registered on field corn and cotton in 1975, soybeans in 1976, tobacco, potatoes, and grain sorghum in 1980, peanuts, sunflowers, and rice in 1981, edible beans and sweet corn in 1984, and sugarcane in 1993. Common name was changed from penoxalin to pendimethalin in 1976.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): BASF; Dow AgroSciences; Helena; Independent Agribusiness Professionals, Inc.; Loveland; Scotts; Tenkoz; Winfield

Reference(s):

1. Moss, S.R. 1990. Weed Sci. 38:492.
2. Mudge, L. C. et al. 1984. Weed Sci. 32:591.
3. Sprankle, P. L. 1974. Proc. 12th Br. Weed Control Conf. 2:825.
4. Vaughn and Lehnen. 1991. Weed Sci. 39:450.
5. Vaughn K.C. et al. 1987. Plant Physiol. 83:956.
6. Vaughn, K. C. et al. 1990. Weed Technol. 4:157.
7. Zimdahl, R. L. et al. Weed Sci. 32:408.

penoxsulam

CAS #: 219714-96-2 **2$^{(B)}$**

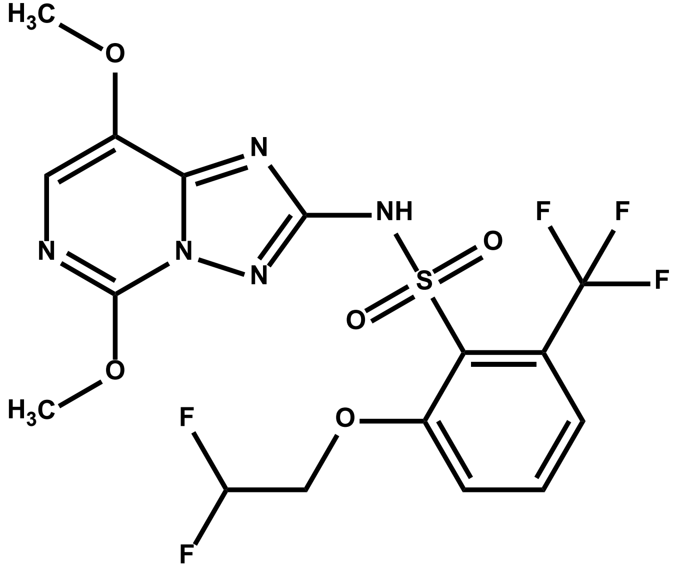
2-(2,2-difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]
pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide
(trifluoromethyl)benzenesulfonamide

NOMENCLATURE

Common name: penoxsulam (ISO provisionally approved)
Other name(s): DE-638; XDE-638; XR-638; DASH-001; DASH-1100; 2-(2,2-difluoroethoxy)-N-5,8-dimethoxy[1,2,4] triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluorotoluene-2-sulfonamide (IUPAC)
Trade name(s): single active: BENGALA™ SC; BOA™ 20 OD; CLIPPER™ 25 OD; FENCER™ OD; GALLEON™ SC; GRANITE™ SC; GRASP™ SC; RAINBOW™ 20 OD; RICER ™SC; SAPPHIRE® ; VIPER™ OD; WIDE ATTACK™ SC; granular formulations: GRANITE™ GR; WIDE ATTACK D GR; premixes: FALKON™ OD; PINDAR™ GT; REBEL EX™**;** TOPSHOT 60 OD, GRASPXTRA SC
Chemical family: sulfonamide; triazolopyrimidine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
penoxsulam



Molecular formula: $C_{16}H_{14}F_5N_5O_5S$
Molecular weight: 483.37 g/mole
Description: Light tan liquid
Density: 1.61 g/mL (20 C)
Melting point: 212 C
Boiling point: NA
Vapor pressure: 2.49 x 10^{-14} Pa (20); 9.55 x 10^{-14} Pa (25 C); Henry's Law constant, 1.66 x 10^{-16} atm m^3/mole (25 C) (estimated)
Stability: Hydrolytically stable in pH 5 to 9 water; thermally stable at typical use temperatures
Solubility:
water 5.7 mg/L (pH 5, 19 C); 410 mg/L (pH 7, 19 C); 1460 mg/L (pH 9, 19 C)
pK$_a$: NA
K$_{ow}$: log K_{ow} = -0.354

HERBICIDAL USE

Penoxsulam provides broad spectrum pre and postflood, postemergence and in-water weed control of susceptible grass, broadleaf, and sedge weeds in rice. It has demonstrated excellent postemergence control with residual activity on Echinochloa grasses. Penoxsulam controls propanil-, quinchlorac- and ACCase-resistant Echinochloa spp. as well. Penoxsulam provides postemergence control with residual activity of many broadleaf and sedge weeds in rice. It is used in transplanted, dry-seeded and water-seeded rice cultures at 10 to 50 g ai/ha. Penoxsulam also controls many important broadleaf weeds and annual sedges commonly found in cool and warm season turfgrass including Bellis, Hydrocotyle, Stellaria, Geranium, Trifolium and Kyllinga species. For turf uses, it is commonly impregnated on granular fertilizer alone, or in combination with other active ingredients. Penoxsulam is also used as an aquatic herbicide to control various submerged weeds including Hydrilla, Eichhornia and Myrophyllum species. Penoxusulam is used in cereals to control certain grass and broadleaf weeds.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: Stable under normal storage conditions
Cleaning glassware/spray equipment: NA
Emergency exposure: Could cause eye irritation; use safety goggles when working with this material. Flush eyes with water; remove contact lenses after initial 1-2 min, and then continue flushing for several minutes. Only mechanical effects are expected. Wash skin with water. If ingested, call a poison control center or doctor immediately for treatment advice. Have person sip a glass of water if able to swallow. Do not induce vomiting unless told to do so by the poison control center or doctor. Never give anything by mouth to an unconscious person. If inhaled, move person to fresh air; if effects occur, consult a physician.
Incompatibilities: Reactivity but no significant rise in temperature for potassium permanganate; non-reactive toward monoammonium phosphate, zinc and water

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Susceptible plant injury from a foliar application of penoxsulam is typical of an ALS inhibitor herbicide and will generally result in growth inhibition, chlorosis at the growing point with possibly some vein reddening, necrosis of the terminal bud in approximately 7 to 14 d after application, and plant death in 2 to 4 weeks.

Absorption/translocation: Penoxsulam is a systemic, phloem-and xylem-mobile herbicide that is absorbed by leaves, shoots, and roots. Penoxsulam is translocated in plants to meristematic tissue.

Metabolism in plants: O-dealkylation of heterocycle methoxy.

Non-herbicidal biological properties: NA

Mechanism of resistance in weeds: ALS enzyme and metabolic resistance.

BEHAVIOR IN SOILS

Sorption: Penoxsulam is weakly adsorbed to soil, but has low leaching potential in most rice soils due to rapid degradation. Fine-textured soils and those high in organic content will bind penoxsulam to a greater extent than coarse/medium soils low in organic matter. High pH soils (pH > 8.0) increase the risk for injury, due to pH-dependent water solubility.

K_{oc}: 104 mL/g

Transformation: Dissipation occurs primarily through microbial degradation.

Photolysis Indirect photodegradation with OH radicals was estimated to be 2.1 h.

Persistence: Penoxsulam is rapidly degraded with half-lives of 5 to 16 days under flooded field conditions.

Mobility: Potential for mobility in soil is high based on K_{oc} values between 50 and 150 mL/g

Volatilization: Penoxsulam is relatively non-volatile due to a low vapor pressure.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade penoxsulam unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, > 5000 mg/kg; Dermal rabbit LD_{50}, >5000 mg/kg; 4-h inhalation LC_{50} rat, >3.5 mg/L; Skin irritation rabbit, very slight, transient irritation; Eye irritation rabbit, mild ocular irritation that cleared within 72 h; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Acute neurotoxicity

Rat study: NOEL > 2000 mg/kg/d

Subacute toxicity:

4-week dermal toxicity, rat: NOEL 1000 mg/kg/d

Subchronic toxicity:

90-d dietary, mouse: NOEL 10 mg/kg/d

90-d dietary, rat: NOAEL 50 mg/kg/d

90-d dietary, dog: NOEL 18 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 10 mg/kg/d not oncogenic

24-mo dietary, rat: NOAEL 5 mg/kg/d not oncogenic

12-mo dietary, dog: NOEL 15 mg/kg/d

1 year chronic neurotoxicity, rat: NOEL 250 mg/kg/d

Teratogenicity:

Rat: NOEL 500 mg/kg/d (maternal); NOEL 1000 mg/kg/d (embryo-fetal); not teratogenic

Rabbit: NOEL 25 mg/kg/d (maternal and embryo-fetal); not teratogenic

Reproduction:

Rat: NOEL 100 mg/kg/d for reproductive tox; 30 mg/kg/d for parental tox

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGTRT, negative; chromosome aberration, negative; in vivo micronucleus, negative; mouse lymphoma assay, negative

DNA damage/repair: NA

Wildlife

Bobwhite quail oral, LD_{50}, >2025 mg/kg; 8-d dietary LC_{50}, >5063 mg/L; chronic NOEL 1000 mg/kg diet Mallard duck oral LD_{50}, >2000 mg/kg; 8-d dietary LC_{50}, >5063 mg/L; chronic NOEL 1000 mg/kg diet Earthworm LC_{50} (14-d), >1000 mg/kg; Honey Bee oral LD_{50}, >100 µg/bee; contact LC_{50}, >100 µg/bee; Seedling emergence (onion) EC_{25}, 1.4 g/ha; Vegetative Vigour (soybean) EC_{25}, 4.2 g/ha; Daphnia 48-h EC_{50}, >98.3 mg/L; 21-d NOEC, 2.95 mg/L; Bluegill sunfish 96-h LC_{50}, >103 mg/L; Rainbow trout 96-h LC_{50}, >102 mg/L; Common carp 96-h LC_{50}, >101 mg/L; Fathead minnow 36-d ELS NOEC, 10.2 mg/L; Eastern oyster 96-h EC_{50}, >127 mg/L; Mysid 96-h EC_{50}, 114 mg/L; Silverside 96-h LC_{50}, 129 mg/L; Nonvascular aquatic plants 96-h EC_{50}, 0.092 mg/L; Vascular aquatic plants 14-d EC_{50}, 0.003 mg/L.

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Residues of penoxsulam are extracted from the crop samples by homogenizing and shaking with an acetonitrile/water solution (80:20 v/v). An aliquot is diluted with 0.1 N HCl and purified using a 96-well polymeric-reverse phase extraction (SPE) plate. The SPE plate is washed with a methanol/water (40:60) solution and eluted with acetonitrile into a 96-well plate containing an acetonitrile/methanol/water mobile phase (15: 15:70) solution containing 0.1% acetic acid and a stable isotope internal standard. The final solution is analyzed by liquid chromatography with positive-ion electrospray tandem mass spectrometry (LC-MS/MS).

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

References:

1. Bioorganic & Medicinal Chemistry (2009), 17(12), 4230-4240.
2. 42nd Central Regional Meeting of the American Chemical Society, Abstracts, June 8-10 (2011), CERM-349

phenmedipham

CAS #: 13684-63-4 $5^{(C_1)}$

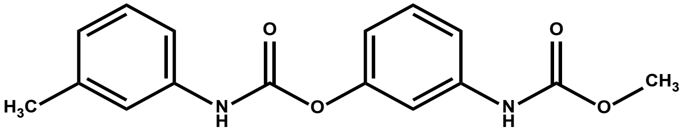
3-[(methoxycarbonyl)amino]phenyl (3-methylphenyl) carbamate

NOMENCLATURE

Common name: phenmedipham (ANSI, BSI, ISO, WSSA)
Other name(s): EP-452; SN 38584; phenmedipháme; methyl 3-(3-methylcarbaniloyloxy)carbanilate or 3-methoxycarbonylaminophenyl 3-methylcarbanilate (IUPAC)
Trade name(s): BETAMIX®; PROGRESS®; PROGRESS® BETA; SPIN-AID®
Chemical family: carbanilate; phenylcarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
phenmedipham



Molecular formula: $C_{16}H_{16}N_2O_4$
Molecular weight: 300.31 g/mole
Description: Colorless, crystalline solid
Density: NA
Melting point: 143-144 C (pure); 140-144 C (technical)
Boiling point: NA
Vapor pressure: 1.33 x 10^{-3} Pa (25 C)
Stability: Stable up to 200 C
Solubility:
water >10 mg/L (20 C)
organic solvents g/100 mL (20 C):

acetone ~20	cyclohexanone ~20
benzene ~0.25	methanol ~5
chloroform ~2	

pK_a: None (non-ionizable)
K_{ow}: 3890 (pH 4)

HERBICIDAL USE

Phenmedipham can be applied POST at 0.41-0.68 kg ai/ha in sugarbeets for control of certain broadleaf weeds.

USE PRECAUTIONS

Fire hazard: BETAMIX is flammable; flash point is 74 C (TCC)
Corrosiveness: Non-corrosive
Storage stability: Phenmedipham has a shelf life of >1 yr
Cleaning glassware/spray equipment: Rinse equipment with water and detergent. Rinse glassware with acetone.
Emergency exposure: If ingested, induce vomiting. High doses could cause hyperactivity, tremors, and muscle spasms.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Leaves appear water-soaked within a few days after application. Chlorosis and necrosis follow soon thereafter.
Absorption/translocation: Readily absorbed by foliage, but poorly translocated in the phloem to other plant parts (2). Rain falling within a few h of application may reduce efficacy.
Metabolism in plants: Phenmedipham hydroxylation and glycosylation followed by hydrolysis of the carbamate linkage appeared to be major factors in sugarbeet tolerance (4). Several metabolites have been identified including a sulfate conjugate (3), but metabolism varies with species (5); the bacterial enzyme phenmedipham hydrolase, coded by a plasmid gene (*pcd*), catalyzed hydrolysis of the carbamate linkage of phenmedipham (8)
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil
K_{oc}: Average is 2400 mL/g (9)
Transformation: Hydrolyzed microbially to 3-aminophenol which complexes with soil.
Persistence: Average field half-life is ~25-30 d (9)
Mobility: No appreciable leaching; phenmedipham remains in the top 5 cm of soil.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade phenmedipham unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat and mouse, >8000 mg/kg; dog and guinea pig, >4000 mg/kg; Dermal LD_{50} rat, >4000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA
BETANAL: Oral LD_{50}, 2000 mg/kg; Dermal LD_{50} rat, >20,000 mg/kg, rabbit, >10,000 mg/kg
Subchronic toxicity: NA
Chronic toxicity:
24-mo dietary, rat: NOEL NA; no histomorphologic alterations at ≤500 mg/kg
24-mo dietary, dog: NOEL 1000 mg/kg/d
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife:
Bobwhite quail 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck oral LD_{50}, >2100 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Chicken oral LD_{50}, >3000 mg/kg; Daphnia 48-h LC_{50}, 3.2 mg/L; Bluegill sunfish 96-h LC_{50}, 3.98 mg/L; Rainbow trout 96-h LC_{50}, 1.4-3 mg/L
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Recrystallization

Analytical methods: Product analysis by titration or by HPLC. Residues in plants are analyzed by GLC (7), and in soil by HPLC or by hydrolysis to *m*-toluidine with derivatives determined by GLC with ECD or by colorimetry (6).

Historical: First tested in Europe in 1966. First reported in 1967 (1). Introduced by Schering AG; British patent 1,127,050. U.S. patents 3,404,075 and 3,692,820.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Arndt and Kotter. 1967. Abstr. 6th Intern. Congr. Plant Prot. Vienna, p. 433.
2. Bromilow and Chamberlain. 1991. Pages245-284 *in* R. C. Kirkwood, ed., Target Sites for Herbicide Action. Plenum Press, New York.
3. Celorio, J. I. et al. 1987. Pesticide Science and Biotechnology: Proc. Sixth Intern. Congr. Pestic. Chem., p. 495.
4. Davies, H. M. et al. 1990. Weed Sci. 38:206.
5. Kassenbeer, H. 1970. Z. Pflanzenkrankh. Pflanzenpath. Pflanzenschutz. 77.
6. Kossmann, K. 1970. Weed Res. 10:340.
7. Kossmann and Jenny. 1973. Anal. Meth. Pestic. Plant Growth Regul. 7:611.
8. Pohlenz, H. O. et al. 1992. J. Bacteriol. 174:6600.
9. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

picloram

4-amino-3,5,6-trichloro-2-pyridinecarboxylic acid

CAS # Acid: 1918-02-1
Isooctyl (2-ethylhexyl) ester: 26952-20-5
Potassium salt: 2545-60-0
Triisopropanolamine salt: 6753-47-5

$4^{(O)}$

NOMENCLATURE

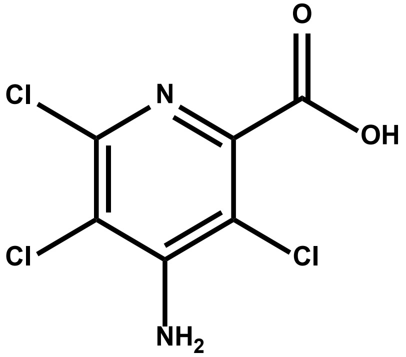
Common name: picloram (ANSI, BSI, E-ISO, JMAF, WSSA)
Other name(s): piclorame (F-ISO); 4-amino-3,5,6-trichloropicolinic acid; 4-amino-3,5,6-trichloropyridine-2-carboxylic acid (IUPAC)

Trade name(s): ALLIGARE PICLORAM + D RTU; ALLIGARE PICLORAM+D; FORESTRY TORDON® 101 MIXTURE; GRAZON® HL; GRAZON® P+D; GRAZON®; HIREDHAND® P+D; MANPOWER® HERBICIDE; OUTLAW®; OUTPOST® 22K; PATHWAY®; PD 2; PICLORAM + 2,4-D RANGELAND; PICLORAM + 2,4-D IVM; PICLORAM + 2,4-D RTU; PICLORAM 10.2 HERBICIDE; SURMOUNT®; TORDON® K; TORDON® 22K;, TORDON® 101 MIXTURE; TORDON® 101R; TORAM® 101; TORDON® RTU; TROPPER® EXTRA SELECTIVE HERBICIDE; TROOPER® PRO HERBICIDE

Chemical family: picolinic acid; pyridinecarboxylic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
picloram



Molecular formula: *Acid* $C_6H_3Cl_3N_2O_2$; *K salt* $C_6H_2Cl_3KN_2O_2$; *Triisopropanolamine (TIPA) salt* $C_{15}H_{24}Cl_3N_3O_5$
Molecular weight: *Acid* 241.46 g/mole; *Io (comment: need to spell out) ester* 353.68 g/mole; *K salt* 279.55 g/mole; *TIPA salt* 432.73 g/mole
Description: White powder, chlorine-like odor
Density: NA
Melting point: Decomposes before melting
Boiling point: NA
Vapor pressure: *Acid* 8.2×10^{-5} Pa (35 C); 1.4×10^{-4} Pa (45 C)
Stability: Decomposed by UV light; decomposes at ~215 C; stable to hydrolysis
Solubility:
Acid
water 430 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 1.98 ethanol 1.05
acetonitrile 0.16 isopropanol 0.55
benzene 0.02 kerosene 0.001
carbon disulfide <0.005
methylene chloride 0.06
diethyl ether 0.12
Potassium and triisopropylamine salts
water 200,000 mg/L (25 C) (estimated) (10)
pK_a: 2.3 (22 C) (weak acid)
K_{ow}: 1.4 (pH 7); 83.2 (pH 1)

HERBICIDAL USE

Picloram can be applied as follows: foliar-applied at 0.14-1.12 kg ae/ha in forest plantings, wildlife openings in forests, non-crop areas such as roadside, railroad, utility, communication rights-of-way, pipelines and industrial sites, and; POST at 0.125-0.56 kg ae/ha in pasture and rangeland; POST at 0.125-0.56 kg ae/ha on Conservation Reserve Program (CRP) land; POST at 0.125-0.28 kg ae/ha in fallow; cut surface (stump, tree injection, and frill or girdle) treatments for woody species using undiluted PATHWAY or TORDON RTU; Picloram controls certain annual broadleaf weeds at low rates and many annual and perennial broadleaf weeds, vines, and woody plants at higher rates. Grass weeds are not controlled. GRAZON P+D can be mixed with certain liquid fertilizers.

USE PRECAUTIONS

Fire hazard: All products are non-flammable; flash points for TORDON 101 MIXTURE and GRAZON P+D are 46 C (TCC), for PATHWAY and TORDON RTU are 41 C (TCC). No flash point was observed for TORDON K and TORDON 22K up to 101 C (TCC).
Corrosiveness: Slightly corrosive to mild steel after prolonged exposure at high temperatures; noncorrosive to other metals.
Storage stability: If picloram formulations are exposed to subfreezing temperatures, they should be warmed to at least 4 C and agitated before using. Store above -2 C or warm and agitate before use.
Cleaning glassware/spray equipment: Rinse equipment three times with ammonia solution. Picloram residues are difficult to remove completely from spray equipment and low concentrations are phytotoxic to susceptible species. Thus, a sprayer used to apply picloram should not be used to spray foliage of susceptible plants.
Emergency exposure: Flush eyes with water for 15 min; consult a physician. Flush skin with water. Induce vomiting if large amounts are ingested; consult a physician.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of Action: is a systemic, ambi-mobile growth-regulator herbicide. (more details on page 12)
Symptomology: Symptoms of picloram injury are typical of

other auxin-type herbicides, and include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 3-5 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.

Absorption/translocation: Readily penetrates roots or foliage with foliar treatments. In sunflowers and rapeseed, 97% of foliar-applied picloram was absorbed within 24 h of application (6). Picloram movement across the plasmalemma may involve both an active protein-mediated process and passive diffusion (1). Picloram is transported rapidly in plant tissues primarily via the symplastic pathway (including the phloem), eventually accumulating at the growing points (9). Over 60% of picloram absorbed by leaves of sunflowers and rapeseed moved out of the treated leaf within 6 d of application (6). Picloram also translocates significantly with the flow of water in the apoplasm (8). Approximately 3% of foliar-applied picloram accumulated in roots of sunflowers and rapeseed (9) and in horsenettle (5).

Metabolism in plants: Picloram metabolism appears to be slow in susceptible species, but more rapid in tolerant ones. Essentially no picloram metabolites were detected 16 d after treatment in horsenettle (susceptible) (5), and only 17% of the picloram absorbed by leafy spurge (susceptible) was metabolized 4 d after application. Most metabolites are water-soluble and suspected to be sugar conjugates (6). Picloram conjugates with glucose in sunflowers to form an *N*-glucoside (3). Leafy spurge metabolized picloram to isomeric glucose esters, gentiobiose esters, and *N*-glucosides (4).). These conjugates have been shown to be readily hydrolyzed back to picloram during laboratory investigations

Non-herbicidal biological properties: As an auxin replacement for growth promotion in cell culture

Mechanism of resistance in weeds: Resistance has developed in a biotype of wild mustard from Canada and in yellow starthistle in Southeastern Washington. The resistance mechanism is unknown, but is a recessive trait and may involve an altered auxin receptor site.

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BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to OM and certain clays, with somewhat greater adsorption to OM. Adsorption to soil increases as level of OM and clay increase.

K_{oc}: Average is 16 mL/g for the K salt (10), but ranges from 17-160 mL/g

K_d: 0.5 mL/g

Transformation:

Photodegradation: Rate of photodegradation is highest in clear, moving water and on soil and plant surfaces. Photolysis half-life in natural water is <2-days and involves cleavage of the pyridine ring.

Other degradation: Degraded somewhat slowly, primarily by aerobic microbial metabolism, resulting in CO_2 as an end-product metabolite. Subsequent degradation of primary degradation products is rapid, leaving only trace amounts of primary products.

Persistence: Average field half-life is 90 d (10), with a range of 20-300 d. Dissipation is more rapid under warm, humid conditions of the southeastern and south central U.S. than in the cool, dry conditions of the northern U.S. Picloram dissipates more rapidly in the presence of plant roots, with higher soil OM content, and at picloram concentrations less than 1.0 lb ae/A. Recent studies at low applications rates showed dissipation half-lives of about 30-days under conditions with sufficient soil moisture.

Lab experiments: Half-lives were 23, 63, and 172 d for picloram at 2.5, 25, and 250 mg/kg, respectively, at 25 C with optimum moisture. Additional studies at normal field application rates (<0.4 mg/kg) yielded half-lives from 5 to 30 d.

Mobility: Highly leachable in some situations, although most picloram residues remain in the top 61 cm of the soil profile. Leaching potential is greatest in sandy soils low in OM, and is affected by other soil and environmental factors as well as by application rate.

Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade picloram acid unless otherwise indicated.

Acute toxicity:

Picloram acid: Oral LD_{50} male rat >5000 mg/kg, female rat 4012 mg/kg, mouse 2000-4000 mg/kg, rabbit ~2000 mg/kg, guinea pig ~3000 mg/kg, sheep >1000 mg/kg, cattle >750 mg/kg; Dermal LD_{50} rabbit >2000 mg/kg; 4-h Inhalation LC_{50} rat >0.035 mg/L; Skin irritation rabbit, none; Skin sensitization Guinea pig, no; Eye irritation rabbit, moderate

Picloram K salt technical: ral LD_{50} male rat, >5000 mg/kg, female rat, 3536 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >1.6 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, moderate

Picloram triisopropanolamine (TIPA) salt technical: Rat LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >0.071 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, minimal

Subchronic toxicity:

90-d dietary, mouse: NOEL <1000 mg/kg/d for the technical acid and K salt; reversible liver effects

90-d dietary, rat: NOEL 50 mg/kg/d for the technical acid and K salt; NOEL 73 mg/kg/d for the technical Io ester; kidney and liver weight increase; NOEL 90 mg/kg/d for the technical TIPA salt

90-d dietary, dog: NOEL 250 mg/kg/d for the technical acid and K salt; increased liver weight

Chronic toxicity:

24-mo dietary, mouse: Systemic NOEL 1000 mg/kg/d; not oncogenic

24-mo dietary, rat: NOEL 20 mg/kg/d; not oncogenic

12-mo dietary, dog: NOEL >175 mg/kg/d; not oncogenic

Teratogenicity:

Rat: NOEL >400 mg/kg/d for the technical acid and K salt; not teratogenic; NOEL 1000 mg/kg/d for the technical Io ester and TIPA salt; not teratogenic

Rabbit: NOEL >400 mg/kg/d for the technical acid and K salt; not teratogenic; NOEL 500 mg/kg/d for the technical isooctyl ester; not teratogenic; NOEL 1000 mg/kg/d for the technical TIPA salt; not teratogenic

Reproduction:

Rat: NOEL parental 200 mg/kg/d, reproductive 1000 mg/kg/d; not a reproductive toxin; renal effects

Mutagenicity:

Gene mutation: Ames test, negative for the technical acid, K salt, Io ester, and TIPA salt; CHO, negative for the technical Io ester and TIPA salt

Structural chromosome aberration: *In vitro* cytogenetics, negative for the technical acid, K salt,; Mouse micronucleus, negative for the TIPA salt

DNA damage/repair: UDS, negative

Wildlife:

Picloram acid: Bobwhite quail 8-d dietary LC_{50}, >5000 mg/kg; Long-term reproductive NOEC, 750 mg/kg; Japanese quail 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Pheasant 8-d dietary LC_{50}, >5000 mg/kg; Earthworm acute LC_{50}, >5000 mg/kg; Honey bee oral LD_{50}, >74 µg/bee; topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50} , 34.4-76 mg/L; Bluegill sunfish 96-h LC_{50}, 14.5-19.4 mg/L; Fathead minnow 96-h LC_{50}, 55.3 mg/L; Rainbow trout 96-h LC_{50}, 5.5-19.3 mg/L; green algae 96-h EC_{50}, 36.9 mg/L

Picloram K salt technical: Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >5620 ppm; Mallard duck oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >10000 mg/kg; Honey bee topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 68.3 mg/L; 21-d NOEC, 11.8 mg/L; Bluegill sunfish 96-h LC_{50}, 24 mg/L; Rainbow trout 96-h LC_{50}, 13 mg/L; ELS NOEC, 0.55 mg/L

Picloram TIPA salt technical: Bobwhite quail 8-d dietary LC_{50}, >10000 mg/kg; Mallard duck 8-d dietary LC_{50}, >10000 mg/kg; Honey bee topical LD_{50}, >100 µg/bee; Daphnia 48-h EC_{50}, 125 mg/L; Mysid shrimp 96-h EC_{50}, 306 mg/L; Bluegill sunfish 96-h LC_{50}, 109 mg/L; Fathead minnow 96-h LC_{50}, 150 mg/L; Rainbow trout 96-h LC_{50}, 375 mg/L

Use classification: Picloram Ready to Use (RTU) products such as PATHWAY or TORDON RTU are General use. All other picloram formulations are Restricted Use Products due to potential injury to susceptible non-target plants.

ANALYTICAL METHODS

Analytical methods: Product is analyzed using infrared at 10.04 µm. Residue analysis (chemical assay) for water samples with a test sensitivity of 0.051 µg/L is available (GRM 00.17, Dow AgroSciences, January 31, 2001)ACR 68:14, Dow, September 26, 1968). Residue analysis for soil samples with a sensitivity of 0.5 µg/kg is available (ACR 73.3, Dow, May 21, 1973120612, Dow AgroSciences, February 20, 2013). Residue analysis for crop tissue samples with a sensitivity of 0.01 µg/g is available (GRM 03.06, Dow AgroSciences, May 1, 2003).

Historical: Picloram was discovered in 1960 and first reported in 1963 (7); introduced by Dow Chemical Company as TORDON 101 in 1963, as TORDON 22K in 1964, as TORDON K in 1972, as TORDON RTU in 1979, and as ACCESS 1982. U.S. patent 3,285,925 was awarded to Dow in 1966.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

Reference(s):

1. Ashton, F. M. and A. S. Crafts. 1981. Mode of Action of Herbicides, 2nd ed. Wiley-Interscience, New York.
2. Chang and Foy. 1983. Pestic. Biochem. Physiol. 19:203.
3. Chkanikov, D. I. et al. 1983. Fiziol. Rast. (mosc) 30(1):95.
4. Frear, D. S. et al. 1989. J. Agric. Food Chem. 37:1408.
5. Gorrell, R. M. et al. 1988. Weed Sci. 36:447.
6. Hall and Vanden Born. 1988. Weed Sci. 36:9.
7. Laning, E. R. 1963. Down to Earth. 19:3.
8. O'Donovan and Vanden Born. 1981. Can. J. Bot. 59:1928.
9. Radosevich and Bayer. 1979. Weed Sci. 27:22.
10. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
11. Woodburn, K.B. et al. 1989. Environ. Toxicol. Chem. 8:769.

picolinafen

CAS #: 137641-05-5

12$^{(F_1)}$

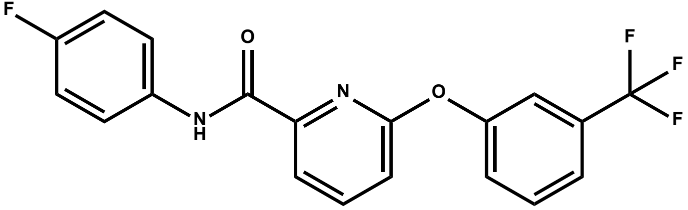
N-(4-fluorophenyl)-6-[3-trifluoromethyl)phenoxy]-2-pyridinecarboxamide

NOMENCLATURE

Common name: picolinafen (ISO 1750 accepted)
Other name(s): 4’-fluro-6-(α,α,α-trifluoro-m-tolyloxy) pyridine-2-carboxanilide (IUPAC)
Trade name(s): SNIPER®
Chemical family: anilide; pyridine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *picolinafen*



Molecular formula: $C_{19}H_{12}F_4N_2O_2$
Molecular weight: 376.31 g/mole
Description: White to chalky-white; finely crystalline solid
Density: 0.24 g/mL
Melting point: 107.2-107.6 C
Boiling point: NA
Vapor pressure: 2.13 x 10^{-5} Pa (20 C)
Stability: Stable
Solubility:
water, 3.9 x 10^{-2} mg/L (20 C)
pK_a: NA
K_{ow}: 2.3 x 10^{-5} (20 C)

HERBICIDAL USE

Picolinafen can be applied PRE and POST up to 100 g ai/ha in wheat, barley, rye and triticale. By controlling broadleaf weeds such as bedstraws (*Galium*), violets (*Viola*) and speedwells (*Veronica*), it provides a complementary activity to other herbicides, allowing effective and broad-spectrum weed control in cereals. At 33-50 g ai/ha, picolinafen is also used for post-emergence control of wild radish (*Raphanus*) in lupins.

USE PRECAUTIONS

Fire hazard: Flammable
Corrosiveness: NA
Storage stability: Stable
Cleaning glassware/spray equipment: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme phytoene desaturase in the carotenoid biosynthesis pathway. (more details on page 14)
Symptomology: Causes bleaching chlorosis of susceptible plant species.
Absorption/translocation: Absorption is faster in susceptible species such as *Sinapis arvensis* than in tolerant species, such as wheat. It is also translocated more extensively within susceptible species.
Metabolism in plants: Not metabolized significantly in plants, both tolerant and susceptible species; differential uptake and translocation accounts for the selectivity between cereals and susceptible weeds.
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: Tightly absorbed to soil particles
K_d: 248 to 764 mL/g
Transformation:
Photodegration: Half-life in water is 23-32 d
Other degradation: Hydrolytically stable
Persistence: Has very little residual soil activity
Field experiments: Half-life in the field is 9 to 64 d with an average of 30 d.
Lab experiments: Aerobic half-life is 1-14 d (20 C). Anaerobic half-life is 7 d.
Mobility: Immobile, being tightly bound to soil particles.
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade picolinafen unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >4000 mg/kg; Dermal irritation rabbit, none; Eye irritation rabbit, none
Formulated product: AC 900001 75% WG: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >4000 mg/kg; Dermal irritation rabbit, none; Eye irritation rabbit, none
Subchronic toxicity:
90-d dietary, mouse: NA
90-d dietary, rat: NA
90-d dietary, dog: 5.2 mg/kg bw/d
Chronic toxicity:
24-mo dietary, rat: 2.4 mg/kg bw/d
12-mo oral capsule, dog: NA
Teratogenicity:
Rat: NA
Rabbit: NA
Reproduction:
Rat: 2-gen rat = 43 mg/kg bw/d
Rabbit: 5 mg /kg bw/d
Mutagenicity:
Gene mutation: CHO/HGPRT, negative
Structural chromosome aberration: NA
Wildlife:
Bobwhite quail and mallard duck oral LD_{50}, >2250 mg/kg;

dietary LC_{50}, >5314 mg/kg; Honey bee oral and dermal LD_{50}, >200 µg/bee; Daphnia 48-h EC_{50}, > 0.45 mg a.s./L; Rainbow trout 96-h LC_{50}, >0.68 mg a.s./L; Earthworm 14-d LC_{50}, >1000 mg/kg

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): BASF

Reference(s):

1. White, R.H., W.S. Clayton, A.F. Burnhams, A. Goldsmith, G. Seaman, T. Walker, H. Baltruschat, F. Schmidt, and J. Weavers. 1999. AC 900001; a new herbicide for broadleaf weed control in cereals. Proc. Br. Crop Prot. Conf.-Weeds. 1:47-52.

pinoxaden

CAS #: 243973-20-8

1(A)

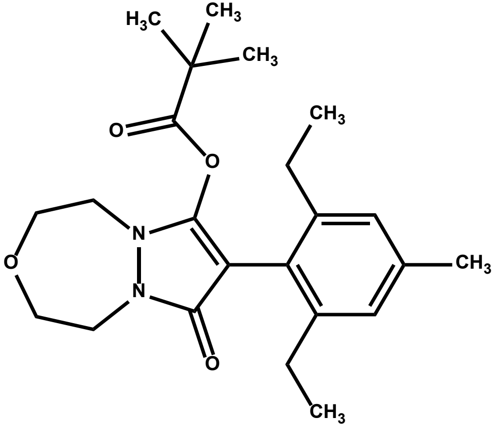
8-(2,6-diethyl-4-methylphenyl)-1,2,4,5-tetrahydro-7-oxo-7H-pyrazolo[1,2-d][1,4,5]oxadiazepin-9-yl 2,2-dimethylpropanoate

NOMENCLATURE

Common name: pinoxaden (ISO-approved)
Other name(s): 8-(2,6-diethyl-p-tolyl)-1,2,4,5-tetrahydro-7-oxo-7H-pyrazolo[1,2-d] [1,4,5]oxadiazepin-9-yl 2,2-dimethylpropionate (IUPAC)
Trade name(s): AXIAL®
Chemical family: phenylpyrazolin

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
pinoxaden



Molecular formula: $C_{23}H_{32}N_2O_4$
Molecular weight: 400.52 g/mole
Description: White fine powder, odorless
Density: 1.16 x 10^3 kg/m^3 (24 C)
Melting point: 120.5-121.6 C
Boiling point: NA
Vapor pressure: 2.0 x 10^{-6} Pa (20 C); Henry's Law constant 9.2 x 10^{-7} Pa m^3 mol^{-1}(20 C)
Stability: Stable at neutral or acidic conditions (half-life 9.9 d (pH 7)); unstable under alkaline conditions.
Solubility: In water, >200 mg/L (25 C)
pK_a: None (non-ionizable)

HERBICIDAL USE

Pinoxaden is active against a broad spectrum of economically important grass weeds including wild oat, foxtails (green, yellow and giant), Italian ryegrass, Persian darnel and barnyardgrass for use on spring wheat (excluding durum), winter wheat and barley. It is sold in mixtures with the safener cloquintocet-mexyl.

USE PRECAUTIONS

Fire hazard: AXIAL™ is a combustible liquid. Vapors can be released that form explosive mixtures at temperatures at or above the flash point. Heave vapors can flow along surfaces to distant ignition sources and flash back. During a fire, irritating and possible toxic gases may be generated by thermal decomposition or combustion.
Corrosiveness: NA
Storage stability: Stable under normal use and storage conditions
Cleaning glassware/spray equipment: Thoroughly clean application equipment immediately after spraying. Ensure that all traces of the product are removed. Drain and flush tank walls, boom, and all hoses for 10 min with clean water. Do not clean the sprayer near desirable vegetation, wells, or other water sources. Remove the nozzles and screens and wash separately. Dispose of all rinsates in accordance with state and local regulations. If a broadleaf herbicide, insecticide, or fungicide tank mix partner is used, always check tank mix partner label for any additional cleanup procedures.
Emergency exposure: Causes moderate eye irritation. Avoid contact wit eyes, skin or clothing; harmful if swallowed or absorbed through the skin. If in eyes, hold eye open and rinse slowly an gently with water for 15-20 min. Remove contact lenses ,if present after the first 5 min, then continue rinsing eye. If on skin or clothing, take off contaminated clothing. Rinse skin immediately with plenty of water for 15-20 min. Call a poison control center or doctor for treatment advice. If swallowed, immediately call a poison control center or doctor. Do not induce vomiting unless told to do so by a poison control center or doctor. Do not give any liquid to the person.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)
Symptomology: Growth ceases within a few days of application with meristematic regions affected first. Leaf chlorosis and eventually necrosis develop within 1-3 wk of application. Leaf sheaths become brown and flaccid at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.
Absorption/translocation: Rapidly absorbed into roots and leaves; translocated predominately in the phloem
Metabolism in plants: Metablolism of pinoxaden has been studied in wheat. The DoR of NAFTA is metabolite M2 (8-(2,6-diethyl-4-methyl-phenyl)-tetrahydro-pyrazolo[1,2-d] [1,4,5]oxadiazepine-7,9-dione), M4 (8-(2,-diethyl-4-hydroxymethyl-phenyl)-9-hydroxy-1,2,4,5-tetrahydro-pyrazolo[1,2-d][1,4,5]oxadiazepin-7-one) and M6 3,5-diethyl-4-(9-hydroxy-7-oxo-1,2,4,5-tetrahydro-7H-pyrazolo[1,2-d] [1,4,5]oxadiazepin-8-yl)-benzoic acid).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Similar to other ACCase-resistant weeds

BEHAVIOR IN SOIL

Sorption: K_{oc}: 299 - 852 mL/g (5 soils)
Transformation:
Photodegradation: Not a significant pathway for

degradation compared to soil metabolis and hydrolysis.

Other degradation: Pinoxaden hydrolyzes with a 10 d half-life in water.

Persistence:

Laboratory experiments: $t_{1/2}$ = <1d in aerobic soil metabolism studies and <1d under anaerobic aquatic conditions.

Field experiments: Pinoxaden was not detected above the limit of quantitation (LOQ) in soil below 0-15 cm depth. The Dt_{50} was ≤ 3d

Mobility: Pinoxaden does not leach

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pinoxaden unless otherwise indicated.

Acute toxicity: Oral LD_{50} rat, > 5000 mg/kg; Dermal LD_{50} rabbit, > 2000 mg/kg; Inhalation (4-h) LC_{50} rat, >5.22 mg/L; Eye contact rabbit, mildly irritating; Skin contact rabbit, moderately irritating but no erythema or edema were noted; Skin sensitizer guinea pig, not a sensitizer

AXIAL® herbicide: Oral LD_{50} rat, > 3129 mg/kg; Dermal LD_{50} rabbit, > 2000 mg/kg; Inhalation (4-h) LC_{50} rat, >5 mg/L; Eye contact rabbit, moderately irritating; Skin contact rabbit, moderately irritating but erythema and edema subsided by day 14, but desquamation was still present; Skin sensitizer guinea pig, not a sensitizer

Subchronic toxicity:

90-day dietary, rat gavage: NOAEL = 300/100 mg/kg/day; LOAEL was not observed in males; = 300 mg/kg/day in females, based on increased water consumption and urinary volume

90-day dietary, rat: NOAEL = 466/537 mg/kg/day; LOAEL – 900/965 mg/kg/day based on decreased body weight and body weight gain and increased incidence of renal lesions in both sexes; decreased food consumption and increased water consumption in males; and increased urine volume in females

90-day dietary, dog: NOAEL = 100 mg/kg/day; LOAEL = 250 mg/kg/day based on clinical signs of toxicity fluid feces, vomit, pale and thin appearance, decreased activity, dehydration, cold to touch, and regurgitation in both sexes, and mucus in feces in the males) and decreased body weights, body weight gains, and food consumption in both sexes

28-day dermal, rat: LOAEL was not observed;
NOAEL = 1000 mg/kg bw/day (the limit dose)

Chronic toxicity:

Dogs: NOAEL = 125 mg/kg/day; LOAEL was not observed

Mouse: NOAEL = 216.5 mg/kg/day (male) and 181.2 mg/kg/day (female)

Neurotoxicity:

No neurotoxic effects (acute or subchronic)

Teratogenicity: NA

Reproduction: Rat: Parental NOAEL = 250 mg/kg/day; Parental LOAEL = 500 mg/kg/day, based on increased water consumption, renal tubular atrophy, and chronic nephropathy in both sexes, and increased incidence of renal pelvic dilation in the males;
Reproductive NOAEL – 500 mg/kg/day; Reproduction LOAEL was not observed

Mutagenicity: NA

Wildlife:

Rainbow trout 96-h LC_{50}, 10.3 mg/L; green algae 72-h EC_{50}, 41 mg/L; Daphnia magna 48-h EC_{50}, 52 mg/L

Use classification: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

pretilachlor

CAS #: 51218-49-6 $15^{(K_3)}$

2-chloro-*N*-(2,6-diethylphenyl)-*N*-(2-propoxyethyl)acetamide

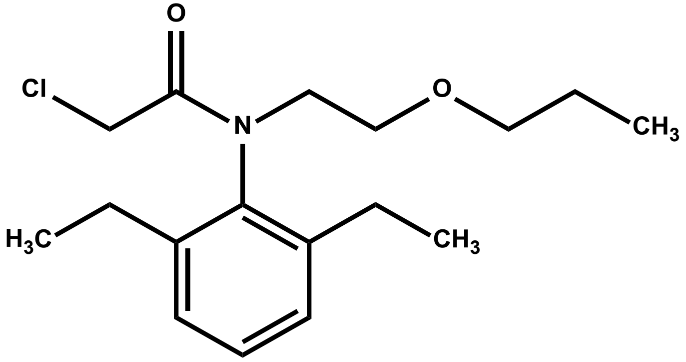
NOMENCLATURE

Common name: pretilachlor (ISO)
Other name(s): prétilachlor (F-ISO); 2-chloro-2',6'-diethyl-*N*-(2-propoxyethyl)acetanilide (IUPAC)
Trade name(s): RIFIT®; SOLNET®; ERIJAN®; SOFIT® (with safener); SOLITO®
Chemical family: acetamide; acetanilide; chloroacetamide; chloroacetanilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

pretilachlor



Molecular formula: $C_{17}H_{26}ClNO_2$
Molecular weight: 311.85 g/mole
Description: colorless liquid
Density: 1.08 g/mL
Melting point: <25 C
Boiling point: 135 C
Vapor pressure: 1.3 x 10^{-4} Pa (20 C)
Stability: 50% hydrolysis occurs in 14 d (pH 13, 20 C)
Solubility: In water, 50 mg/L (20 C). Very soluble in benzene, hexane, methanol
pK$_a$: None (non-ionizable)
K$_{ow}$: log K_{ow} = 4.08

HERBICIDAL USE

Pretilachlor is a chloroacetanilide used for preemergence or early postemergence control of annual grasses and broadleaf weeds in translocated and seeded rice at 0.3 kg ai/ha. Not used on dry seeded rice. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of very long chain fatty acid (VLFCA) synthesis. (more details on page 14)
Symptomology: Inhibition of shoot growth in seedling weeds.
Absorption/translocation: Absorbed by roots; translocated primarily in the xylem
Metabolism in plants: Pretilachlor undergoes conjugation with gluthathione that results in dechlorination. Cleavage of ether linkage also occurs.
Mechanism of resistance in weeds: No resistance reported

BEHAVIOR IN SOIL

Sorption: NA
Transformation: NA
Persistence:
Lab experiments: DT$_{50}$ 20-50 d
Volatilization: Moderately volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pretilachlor unless otherwise indicated.

Acute toxicity:
Oral LD$_{50}$ rat, 6099 mg/kg; Dermal LD$_{50}$ rat, 3mg/kg; Skin irritation, moderate; Eye irritation rabbit, no
Chronic toxicity:
6-mo dietary, dog: NOEL 300 mg/kg
Wildlife:
Slightly toxic to bees, non-toxic to earthworms; rainbow trout LC$_{50}$ (9 h), 0.9 mg/L, catfish, 2.7 mg/L, crucion carp, 2.3 mg/L
Use classification: WHO class V

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Syngenta Crop Protection
Reference(s):

1. Roberts, T. R. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry100

primisulfuron-methyl

CAS #: 86209-51-0 $2^{(B)}$

methyl 2-[[[[[4,6-bis(difluoromethoxy)-2-pyrimidinyl]amino]carbonyl]amino]sulfonyl]benzoate

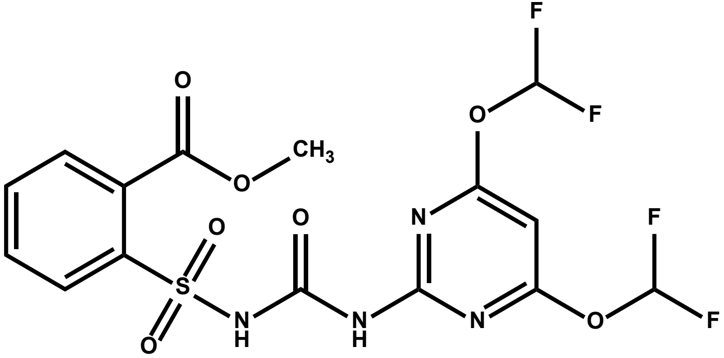
NOMENCLATURE

Common name: primisulfuron-methyl (ANSI, BSI, ISO, WSSA)
Other name(s): CGA-136872; methyl 2-[4,6-bis(difluoromethoxy)pyrimidin-2-ylcarbamoylsulfamoyl]benzoate (IUPAC)
Trade name(s): BEACON®; NORTHSTAR®; SPIRIT®
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure

primisulfuron-methyl



Molecular formula: $C_{15}H_{12}F_4N_4O_7S$
Molecular weight: 468.34 g/mole
Description: Crystalline solid, colorless to yellow, odorless
Density: 1.62 g/mL (20 C)
Melting point: 203 C
Boiling point: NA
Vapor pressure: $< 5 \times 10^{-6}$ Pa (25 C); Henry's Law constant, $<9.5 \times 10^{-11}$ atm m^3/mole
Stability: Hydrolyzes with a half-life of 10 h (50 C) and pH 3
Solubility:
water, 3.3 mg/L (pH 5, 20 C); 243 mg/L (pH 7, 20 C); 5280 mg/L (pH 9, 20 C)
organic solvents g/100 mL (20 C):
acetone 3.6
cyclohexanone 2.7
dichloromethane 0.4
ethanol 0.1
isopropanol 0.04
methanol 0.35
n-octanol 0.0008
toluene 0.05
xylene 0.03
pK_a: 5.1 (weak acid)
K_{ow}: 1.15 (25 C)

HERBICIDAL USE

Primisulfuron can be applied POST at 20-40 g ai/ha in corn. It controls certain annual and perennial grass weeds such as fall panicum, shattercane, johnsongrass, and quackgrass, as well as many annual broadleaf weeds such as pigweed spp., velvetleaf, smartweed, giant ragweed, jimsonweed, cocklebur, and nightshade spp. A surfactant or oil adjuvant is essential for maximum efficacy. Some corn hybrids are susceptible to primisulfuron.

USE PRECAUTIONS

Fire hazard: The product BEACON is nonflammable
Corrosiveness: The product BEACON is non-corrosive; stainless steel, aluminum, fiberglass, or polyethylene are recommended for spray tanks
Storage stability: Stable when stored cool and dry, but stability may decrease when stored under moist conditions; BEACON® remains active in the spray solution for at least 48 h
Cleaning glassware/spray equipment: Clean glassware and spray equipment with 2% v/v ammonia. Use a pressure rinser to direct the ammonia solution inside the spray tank. Clean nozzles and screen separately
Emergency exposure: If ingested, induce vomiting or lavage stomach. No specific antidote is available, but a slurry of activated charcoal may help adsorb ingested primisulfuron.
Incompatibilities: Certain organophosphate insecticides (especially terbufos) applied at planting or tank mixed with primisulfuron may inhibit rapid metabolism of POST-applied primisulfuron, resulting in corn injury. POST application of an organophophate insecticide within 10 d before or 7 d after primisulfuron application may result in crop injury. Primisulfuron applied in a liquid fertilizer carrier may result in crop injury.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Growth is rapidly inhibited in susceptible species, resulting in stunted plants. Foliar chlorosis begins to appear within 5-7 d, followed by chlorosis and necrosis of the growing point of broadleaves, and foliar necrosis. Veins on the underside of leaves are discolored, often reddish purple. Root growth inhibition sometimes occurs. Complete plant death may require 14-21 d
Absorption/translocation: Readily absorbed by both foliage and roots, and translocates primarily in the phloem. When applied to leaves, primisulfuron translocates to shoot growing points and at moderate levels to the roots. Root-absorbed primisulfuron translocates efficiently to all parts of the shoots, including meristematic areas.
Metabolism in plants: Primisulfuron is detoxified rapidly in corn by hydroxylation at the phenyl and at the pyrimidine ring by cytochrome P450 monooxygenases (2). The ring hydroxyl groups are subsequently conjugated with glucose. A relatively minor reaction involves hydrolytic cleavage of the sulfonylurea bridge yielding CO_2, a pyrimidine amine metabolite, and a benzenesulfonamide metabolite.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Sulfonylurea-resistant weed biotypes in a few species have been selected in the

field by chlorsulfuron use. The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil

K_{oc} and K_d: K_{oc} is 50 mL/g (estimated) (1). K_d <0.01 mL/g for a sand with 4.8% OM, 2.2% clay, and pH 6.5; K_{oc} 4.0 mL/g and K_d 0.04 mL/g for a sandy loam with 0.9% OM, 16.8% clay, and pH 7.5; K_{oc} 20.0 mL/g and K_d 0.09 mL/g for a loam with 0.8% OM, 9% clay, and pH 6.7; K_{oc}13 mL/g and K_d 0.38 mL/g for a clay with 1.9% OM, 42% clay, and pH 5.9

Transformation:

Photodegradation: At 25 C with natural light, primisulfuron is stable at pH 9, but half-life is 22 d at pH 5, producing saccharin (10.1% of applied) and [benzoic acid, 2-(amino sulfonyl), methylester] (53.3%). Half-life was 24 d in a sandy loam at 25 C under a xenon lamp.

Other degradation: Half-lives were 41-89 d for anaerobic and 30-63 d for aerobic laboratory conditions in a sandy loam soil at 25 C.

Persistence: Moderate residual with an average field half-life of 30 d (1). Residues can persist long enough to injure sugarbeets the following year.

Field experiments: Half-lives in bare ground dissipation studies sampling 0-15 cm: 13 d for a silt loam with 2.5% OM and pH 5.8 in New York; 11 d for a clay loam with 1.8% OM and pH 7.4 in Mississippi; 8.2 d for a silt loam with 2.5% OM and pH 6.8 in Nebraska; 3.9 d for a loamy sand with 3.1% OM and pH 6.1 in Georgia. Application rate and environmental and edaphic conditions can significantly impact half-life.

Mobility: In field experiments conducted in corn grown in Wisconsin and Indiana, no quantifiable primisulfuron residues (LOD = 0.5-1 mg/kg) were found below 30 cm.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade primisulfuron unless otherwise indicated.**Acute toxicity:**

Oral LD_{50} rat, >5050 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >4.8 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

BEACON: Oral LD_{50} rat, >5050 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >3.3 mg/L; Skin irritation rabbit, slight; Skin slight

Subchronic toxicity:

90-d dietary, mouse: NOEL 300 mg/kg; teeth disorders and liver changes at ≥3000 mg/kg; kidney changes at 10,000 mg/kg

90-d dietary, rat: NOEL 24.5 mg/kg/d; teeth disorders and testicular effects at ≥10,000 mg/kg

90-d dietary, dog: NOEL 0.8 mg/kg/d; gall bladder effects at ≥1000 mg/kg; thyroid effects at 10,000 mg/kg

21-d dermal, rabbit: NOEL 1000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: Study 1, NOEL <500 mg/kg; liver changes in both sexes, and testicular degeneration and nephropathy in males at 1500 mg/kg (highest dose tested); not carcinogenic; Study 2, NOEL 1500 mg/kg; increased incidences of hepatocellular adenomas and carcinomas, teeth and bone disorders, chronic nephritis, and testicular degeneration at 3000 and 7000 mg/kg

24-mo dietary, rat: NOEL 300 mg/kg; increased incidence of teeth disorders, chronic nephritis, and testicular atrophy at 8000 mg/kg; not carcinogenic

12-mo dietary, dog: NOEL 25 mg/kg/d; liver effects at 5000 mg/kg

Teratogenicity:

Rat: NOEL 100 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 100 mg/kg/d, developmental 600 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 1000 mg/kg; reduction in fertility indices and testicular effects in parental animals, and lower pup body weights at 5000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; CHO (V79 cells), negative

Structural chromosome aberration: Chinese hamster/ micronucleus, negative; CHO, negative; Chinese hamster/ nucleus anomaly, negative

DNA damage/repair: Rat hepatocyte, negative; Human fibroblast, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Honey bee oral LD_{50}, >100 µg/bee; topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 260 mg/L; Bluegill sunfish 96-h LC_{50}, >180 mg/L; Rainbow trout 96-h LC_{50}, 210 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: A multi-step synthesis starting with thiourea and diethylmalonate, and culminating with the coupling of an aminosulfonyl-benzoic acid with a pyrimidinyl isocyanate

Purification of technical: Recrystallization in xylene and washing with methanol

Analytical methods: Crop samples are extracted by homogenizing with 90% methanol. Extracts are concentrated and made basic with a sodium carbonate/NaCl solution. Residues are partitioned into ethyl acetate. Ethyl acetate is then diluted with hexane and partitioned with a dilute solution. The aqueous fraction is acidified with acetic acid and partitioned with dichloromethane. The dichloromethane fraction is cleaned-up on Alumina A and silica SepPaks. Residues are determined by reverse phase HPLC with UV detection. Soil residues are extracted by shaking in acetonitrile/NH_4OH. Sodium carbonate is added and the solution is partitioned with toluene. The aqueous fraction is then acidified with phosphoric acid and the residues partitioned into dichloromethane. Residues are cleaned-up on an Alumina A SepPak and analyzed by reverse phase HPLC with UV detection. Water residues are extracted by acidification and partitioned with dichloromethane. The dichloromethane fraction is concentrated and primisulfuron is determined by reverse phase HPLC with UV detection at 240 nm.

Historical: Primisulfuron was synthesized and discovered by Ciba-Geigy Ltd, Basel, Switzerland. It was first field tested in 1983 and became commercially available for use on corn in 1990. Herbicidal activity of primisulfuron was first reported in 1987 (4). European patent 84,020 and U.S. patent 4,478,635.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Fonné-Pfister, R. et al. 1990. Pestic. Biochem. Physiol. 37:165.
3. LaRossa and Schloss. 1984. J. Biol. Chem. 259:8753.
4. Maurer, W. et al. 1987. Proc. Br. Crop Prot. Conf. Weeds. 1:41.

prodiamine

CAS #: 29091-21- $3^{(K_1)}$

2,4-dinitro-*N*^{3},*N*^{3}-dipropyl-6-(trifluoromethyl)-1,3-benzenediamine

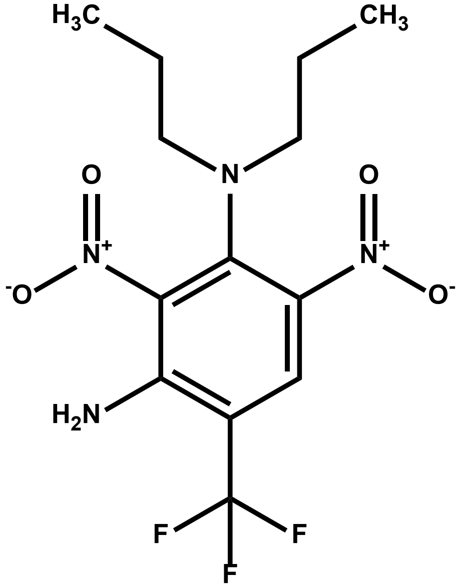
NOMENCLATURE

Common name: prodiamine (ANSI, BSI, ISO, WSSA)
Other name(s): CN-11-2936; SAN-745H; USB-3153; 2,6-dinitro-*N*^{1},*N*^{1}-dipropyl-4-trifluoromethyl-*m*-phenylenediamine or 5-dipropyl-amino-〈,〈,〈-trifluoro-4,6-dinitro-*o*-toluidine (IUPAC)
Trade name(s): BARRICADE®; MARATHON; PRO-MATE®;
Chemical family: dinitroaniline; phenylenediamine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

prodiamine



Molecular formula: $C_{13}H_{17}F_3N_4O_4$
Molecular weight: 350.30 g/mole
Description: Yellow-orange powdered solid
Density: 1.41 g/mL (25 C)
Melting point: 122.5 – 124 C
Boiling point: Decomposes before boiling
Vapor pressure: 3.34×10^{-6} Pa (extrapolated), Henry's Law constant, 8.9×10^{-7} atm m^3/mole
Stability: Decomposes at 240 C; moderately stable to light (dilute solutions degraded by UV light)
Solubility:
  water 0.013 mg/L (25 C)
  organic solvents g/100 mL (20-25 C):
  ethanol 2
pK_a: None (non-ionizable)
K_{ow}: 12,672 ± 2,270 (25 C)

HERBICIDAL USE

Prodiamine can be applied PRE at 0.42-1.7 kg ai/ha in established turf and ornamentals. Prodiamine controls many annual grasses including barnyardgrass, crabgrass spp., fall panicum, foxtails, goosegrass, and seedling johnsongrass, as well as certain annual broadleaf weeds such as lambsquarters, pigweed spp., and prostrate spurge.

USE PRECAUTIONS

Fire hazard: Prodiamine technical and BARRICADE are dry and non-flammable.
Corrosiveness: Prodiamine technical and BARRICADE are non-corrosive.
Storage stability: Stable at ambient temperatures
Cleaning glassware/spray equipment: Rinse glassware with water and detergent, then with acetone. Flush equipment with water and detergent.
Emergency exposure: Rinse eyes with water for 13 min; contact a physician if irritation persists. Wash skin with soap and water. If ingested, drink 1-2 antidote is available.
Incompatibilities: Oxidizing agents (spill control and clean-up)

BEHAVIOR IN PLANTS

Mechanism of action: Mitotic disruption through inhibition of the microtubule protein tubulin (more details on page 12)
Symptomology: Inhibition of root and shoot growth
Absorption/translocation: Emerged and maturing plants translocate little prodiamine from roots and shoots.
Metabolism in plants: Rapidly degraded by plants
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Modification at the site of action

BEHAVIOR IN SOIL

Sorption: Strongly absorbed to soil
  K_{oc}: Average K_{oc} is 13,000 mL/g (1). K_{OC} 19,540 mL/g and K_d 19.54 mL/g for a sand; K_{oc} 12,860 mL/g and K_d 398.5 mL/g for a sandy loam, K_{oc} 5440 mL/g and K_d 120 mL/g for a Kenyon loam
Transformation:
  Photodegradation: Half-life was 50 h for prodiamine at 500 mg/kg and 63 h for prodiamine at 2 mg/kg on a dry Kenyon loam exposed to sunlight at 1000 W/m^2 average intensity (June, Chicago, IL)
  Other degradation: Half-life was 57 d for aerobic metabolism and 30 d for anaerobic metabolism
Persistence: Half-life averages ~ 120 d when incorporated at recommended rates.
  Field experiments: Half-life was 69 d for a sandy loam in Georgia on a turf site.
Mobility: Not readily leached
Volatilization: Losses occur during prolonged exposure on the soil surface without incorporation.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade prodiamine unless otherwise indicated.

Acute toxicity:

Oral LD$_{50}$ rat, >5000 mg/kg, mouse, >5000 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; 4-h inhalation LC$_{50}$ rat, >0.256 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

BARRICADE 65WG: Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; 4-h inhalation LC$_{50}$ rat, >1.8 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, mild

BARRICADE F: Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL 60 mg/kg/d; reduced body weight gains; increased cholesterol in m increased urinary protein at 200 mg/kg/d

90-d dietary, dog: NOEL 200 mg/kg; increased liver weight accompanied by histopathology at 2000 mg/kg

Chronic toxicity:

24-mo dietary mouse: NOEL 500 mg/kg; reduced body weight gains; increased liver weight at 5000 mg/kg

24-mo dietary, rat: NOEL 200 mg/kg; reduced body weight gains; increased thyroid tumors at 3200 mg/kg

12-mo dietary, dog: NOEL 200 mg/kg; liver damage at 2000 mg/kg

Teratogenicity:

Rat: NOEL fetal 100 mg/kg/d, maternal 300 mg/kg/d; decreased maternal body weight gains at 1000 mg/kg; not teratogenic

Rabbit: NOEL fetal 500 mg/kg/d; maternal 100 mg/kg/d; decreased maternal body weight gains at 300 mg/kg/g; not teratogenic

Reproduction:

Rat: NOEL 200 mg/kg; decreased body weight gains; increased liver weights at 2000 mg/kg

Mutagenicity:

Gene mutation: Ames, test, negative

Structural chromosome aberration: CHO, negative

DNA damage/repair: Rat primarily hepatocytes/UDS, negative

Wildlife:

Bobwhite quail oral LD$_{50}$, >2250 mg/kg; 8-d dietary LC$_{50}$, >10,000 mg/kg; Mallard duck 8-d dietary LC$_{50}$, >10,000 mg/kg; Honey bee topical LD$_{50}$, >100 αg/bee; Daphnia 48-h LC$_{50}$, >0.658 mg/L; Bluegill sunfish 96-h LC$_{50}$, >0.552 mg/L; Rainbow trout 96-h LC$_{50}$, >0.829 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 2.4-dichlorobenzotrifluoride is subjected to nitration, dipropylamination, and ammoniation. See U.S. patents 3,617,252 and 3,764,623.

Purification of technical: Technical prodiamine is slurried in cyclohexane, heated under reflux, filtered hot, cooled to room temperatures, recrystallized in isopropanol, and vacuum dried. Two more recrystallizations from 95% ethanol yields >91% active prodiamine.

Analytical methods: Formulated products and technical prodiamine can be assayed for purity by GC-FID using di-n-hexyl phthalate as internal standard (SAI AM-0978-1090-2). Prodiamine in water can be extracted with dichloromethane, cleaned-up with florisil, and quantified by GC-ECD (SAI AM-0792). Prodiamine and the 6-amino-imidazole metabolite in soil can be extracted with methanol followed by dilution with water and partitioning into dichloromethane, silica gel clean-up, and quantification by GC-ECD (SAI AM-0817). Prodiamine and metabolites in tissues can be determined by hydrolysis with 6*N* HCl followed by extraction with dichloromethane for wet tissues or with 1:1 methanol/dichloromethane followed by acetonitrile/hexane partitioning for adipose tissues. Extracts are cleaned-up with gel permeation and florisil chromatography, and quantified with GC-ECD (SAI AM-0805).

Historical: Prodamine was discovered by US Borax (USB-3153), developed by Velsicol Chemical Corporation (Cn-11-2936) and is marketed by Sandoz (SAN-745H). Prodamine was introduced March 18-20, 1975 at the Western Society of Weed Science meetings in Phenix, Arizona.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Agriliance; Helena

Reference(s):

1. Augustijn, Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1. Vaughn and Lehnen. 1991. Weed Sci. 39:450.

prometon

CAS #: 1610-18-0 $5^{(C_1)}$

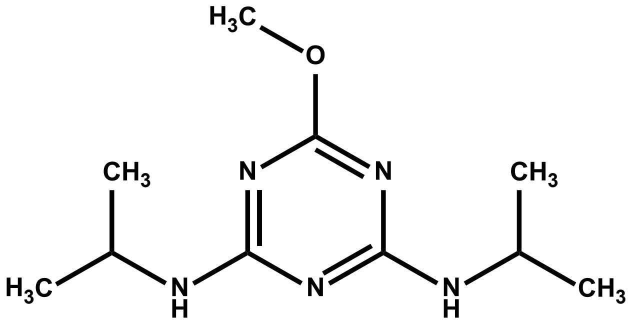
6-methoxy-*N*,*N'*-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: prometon (ANSI, BSI, ISO, WSSA)
Other name(s): G-31435; prometone; *N*,*N*-diisopropyl-6-methoxy-[1,3,5]-triazine-2,4-diamine; N^2,N^4-diisopropyl-6-methoxy-1,3,5-triazine-2,4-diamine (IUPAC); 2,4-bis(isopropylamino)-6-methoxy-*s*-triazine; 4,6-bisisopropylamino-2-methoxy-1,3,5-triazine; 4,6-bis(isopropylamino)-2-methoxy-*s*-triazine; 2-methoxy-4,6-bis(isopropylamino)-*s*-triazine
Trade name(s): ACME®; GESAGRAM; PRAMITOL®; PROMETON®
Chemical family: methoxy-*s*-triazine; methoxy triazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
prometon



Molecular formula: $C_{10}H_{19}N_5O$
Molecular weight: 225.29 g/mole
Description: White crystalline solid
Density: 1.09 g/mL (20 C)
Melting point: 91-92 C
Boiling point: NA
Vapor pressure: 7.8×10^{-5} Pa (10 C); 3.1×10^{-4} Pa (20 C); 10^{-3} Pa (25 C); 3×10^{-3} Pa (40 C); 3.3×10^{-2} Pa (50 C); 6.5×10^{-1} Pa (75 C); 87 Pa (100 C); 83 Pa (125 C); 650 Pa (150 C); Henry's Law constant, 3.19×10^{-9} atm m^3/mole
Stability: Relatively stable at neutral pH, but hydrolyzes in strong acid or base; decomposed by UV light
Solubility:
water 720 mg/L (22 C)
organic solvents g/100 mL (20 C):
acetone 30
benzene >25
cyclohexane 4.9
dichloromethane 35
n-hexane 1.2
methanol 60
n-octanol 26
toluene 34

pK_a: 4.3 (20 C) (weak base)
K_{ow}: 492 (pH 7, 25 C)

HERBICIDAL USE

Prometon is a non-selective herbicide applied PRE or POST at 9-22.4 kg ai/ha on non-crop land (industrial sites, railroad rights of way, underneath asphalt, etc.). Prometon does not control woody species, but controls many annual and perennial grass and broadleaf weeds including downy brome, quackgrass, goldenrod, johnsongrass, bindweed, and wild carrot. It can be applied in water or using diesel fuel or other oils as a carrier.

USE PRECAUTIONS

Fire hazard: The product PROMETON 25E and PRAMITOL 25E are flammable with flash points of 34.4 C. PRAMITOL 1.5% has a flash point of 38.9 C (TCC).
Corrosiveness: PRAMITOL 25E is non-corrosive to metals or equipment.
Storage stability: Stable over several years of dry storage; slightly sensitive to sunlight
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: PRAMITOL 5PS and 25E, and PROMETON 5PS and 25E are corrosive to eyes and irritate skin. If ingested, induce vomiting after drinking 1-2 glasses of water; repeat until vomit fluid is clear. Do not lavage stomach. Treat for circulatory shock, respiratory depression, and convulsions if needed.
Incompatibilities: Compatible with most other pesticides

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Symptoms begin with interveinal chlorosis in the leaves and yellowing of their margins. Older leaves show more injury than new growth. Browning of the leaf tips can occur. In susceptible species, leaves become completely brown and desiccated.
Absorption/translocation: Readily absorbed by foliage and roots. Little to no basipetal movement occurs after foliar absorption. Root-absorbed prometon is translocated primarily in the xylem to all parts of the shoot system, with greatest accumulation in mature leaves.
Metabolism in plants: Prometon is metabolized in tolerant plants to hydroxyprometon. Further metabolism involves *N*-dealkylation of side chains followed by hydrolytic cleavage of resulting amino groups from the triazine ring.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Many species worldwide have developed triazine-resistant biotypes. Those studied at the genetic level have an altered *psbA* gene coding for a glycine in place of a serine on the D1 protein on which the atrazine binding site is located. Thus, triazines cannot bind efficiently to the D1 protein and do not block photosynthetic electron transport. Most of these biotypes have been selected in the field by use of atrazine or simazine, but they appear to be resistant to all triazines including prometon.

BEHAVIOR IN SOIL

Sorption: Prometon is moderately adsorbed, but is more strongly adsorbed on soils high in OM and clay.

K_{oc} and K_d: Average K_{oc} is 150 mL/g (2); K_{oc} 213 mL/g and K_d 0.38 mL/g for a sand with 2% clay, 0.3% OM, and pH 5.4; K_{oc} 90 mL/g and K_d 0.58mL/g for a silt loam with 13% clay, 1.1% OM, and pH 7; K_{oc} 51 mL/g and K_d 0.75 mL/g for a silty clay loam with 28% clay, 2.5% OM and pH 6.6; K_{oc} 103 mL/g and K_d 0.85 mL/g for a silty clay loam with 40% clay, 1.4% OM, and pH 7.8

Transformation:

Photodegradation: Stable in water at 25 C under sunlight. Half-life was 46.8 d on a sandy loam soil at ~25 C under sunlight, producing the mono-*N*-dealkylated metabolite (6-methoxy-*N*-(1-methylethyl)-1,3,5-triazine-2,4-diamine); moderate contribution to field dissipation, especially when lack of rainfall allows prometon to remain on the soil surface

Other degradation: Half-life was 431 d for aerobic metabolism in a sandy loam at 25 C, producing low levels of the mono-*N*-dealkylated metabolite and hydroxy prometon [4,6-bis[(1-methylethyl)amino]-1,3,5-triazine-2(1*H*)-one]. Prometon also is metabolized very slowly under anaerobic conditions in a sandy loam at 25 C. Overall microbial degradation is slow. Prometon is stable in water at pH 5, 7, or 9. Non-microbial hyrolysis rates in soil are negligible.

Persistence: Highly persistent, especially under dry, cool conditions; average field half-life is 500 d (2)

Field experiments: Half-lives in bareground dissipation studies sampling 0-15 cm: 717 d in a silt loam with 2.8% OM and pH 6.3 in New York; 264 d in a sandy loam with 0.7% OM and pH 6.7 in California; 3084 d in a silt loam with 2.9% OM and pH 5.4 in Nebraska

Mobility: Moderately mobile

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade prometon unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 4345 mg/kg; female rat, 1518 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat, >3.26 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

PRAMITOL 25E: Oral LD_{50} rat, 2100 mg/kg; Dermal LD_{50} rabbit, 2000 mg/kg; 4-h inhalation LC_{50} rat, >2.36 mg/L; Skin irritation rabbit, severe; Eye irritation rabbit, corrosive

PRAMITOL 5PS: Oral LD_{50} rat, 3090 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >3.7 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL 15 mg/kg/d (300 mg/kg)

21-d dermal, rabbit: NOEL 25 mg/kg/d; body weight and body weight gain reductions at ≥500 mg/kg/d; slight adrenal gland effects in females at 1050 mg/kg/d

Chronic toxicity:

21-mo dietary, mouse: NOEL 70 mg/kg/d; not carcinogenic; liver, kidney, and spleen effects at 4000 and 8000 mg/kg

24-mo dietary, rat: NOEL 1 mg/kg/d; not carcinogenic; body weights reduced at ≥500 mg/kg

12-mo dietary, dog: NOEL 5 mg/kg/d; increased emesis and lethargy at 20 and 50 mg/kg/d; body weight effects in males at 50 mg/kg/d

Teratogenicity:

Rat: NOEL maternal <36 mg/kg/d, developmental 120 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 3.5 mg/kg/d, developmental 24.5 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 1 mg/kg/d; not a reproductive toxin; body weight effects at 500 and 1500 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Rat micronucleus, negative

DNA damage/repair: Rat hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2264 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, 3158 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Honey bee topical LD_{50}, 36 μg/bee; Daphnia 48-h LC_{50}, 37.5 mg/L; Bluegill sunfish 96-h LC_{50}, 41.5 mg/L; Crucian carp 96-h LC_{50}, 70 mg/L; Rainbow trout 96-h LC_{50}, 19.6 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Successive *N*-alkylations of cyanuric chloride followed by reaction with methanol to attach the methoxy group.

Purification of technical: Recrystallization from toluene

Analytical methods: Crop samples are extracted by reflux in 80% methanol. Residues are partitioned into ethyl acetate/hexane and cleaned-up on a water-deactivated alumina column. Extracts can be analyzed by GC (with N/P detection or MS) or HPLC (with UV-VIS). Prometon is determined in technical samples and formulations using GC with flame ionization detection.

Historical: Synthesis and testing of triazine compounds as herbicides began in 1952 in the Geigy Laboratories in Basel, Switzerland. Prometon was first released for experiment station evaluation in 1958 and became commercially available in 1959. First reported in 1960 (1). Swiss patent 337,019 and British patent 814,948.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Agriliance; Syngenta Crop Protection; Helena; PBI Gordon; UAP-Platte; Riverside/Terra

Reference(s):

1. Gysin and Knusli. 1960. Adv. Pest Control Res. 3:289.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

prometryn

CAS #: 7287-19-6 **5$^{(C_1)}$**

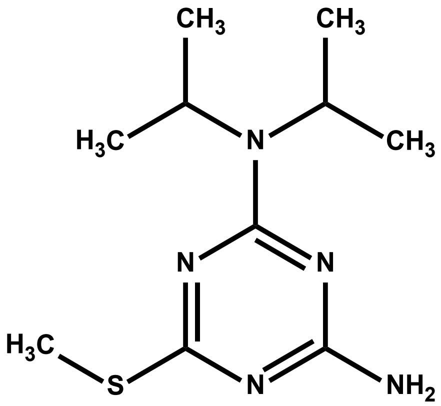
N,*N′*-bis(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: prometryn (ANSI, BSI, ISO, WSSA).
Other name(s): G-34161; prometryne; *N*,*N′*-diisopropyl-6-methyl-sulfanyl-[1,3,5]-triazine-2,4-diamine; *N*^{2},*N*^{4}-diisopropyl-6-methylthio-1,3,5-triazine -2,4-diamine (IUPAC); 2,4-bis(isopropylamino)-6-methylmercapto-*s*-triazine; 2,4-bis(isopropylamino)-6-(methylthio)-*s*-triazine; 2-methylthio-4,6-bis(isopro-pylamino)-*s*-triazine
Trade name(s): CAPAROL®; COTTON PRO®; GESAGARD; VEGETABLE PRO™
Chemical family: methylthio-*s*-triazine; methylthio triazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
prometryn



Molecular formula: $C_{10}H_{19}N_5S$
Molecular weight: 241.35 g/mole
Description: White, crystalline
Density: 1.157 g/mL (20 C)
Melting point: 118-120 C
Boiling point: NA
Vapor pressure: 3.2×10^{-5} Pa (10 C); 1.3×10^{-4} Pa (20 C); 1.6×10^{-4} Pa (25 C), 5.3×10^{-4} Pa (30 C); 2×10^{-3} Pa (40 C); 6×10^{-3} Pa (50 C); Henry's Law constant, 1.19×10^{-8} atm m^3/mole
Stability: DSC endotherm at 110 C, DSC exotherm at ~210 C stable for over 8 h at 170 C; stable in neutral and mildly acidic or basic media, but hydrolyzed in strong acid or base; decomposed by UV light.
Solubility:
water 33 mg/L (22 C)
organic solvents g/100 mL (20 C):

acetone 24	*n*-hexane 0.55
dichloromethane 30	*n*-octanol 10
methanol 16	toluene 17

pK_a: 4.09 (20 C) (weak base)
K_{ow}: 1212 (25 C)

HERBICIDAL USE

Prometryn can be used PPI, PRE, and directed POST in cotton at 0.56-3.1 kg ai/ha, PRE or POST in celery at 0.67-3.6 kg ai/ha, and PRE in pigeon peas at 2.24-3.36 kg ai/ha. Weeds controlled include groundcherry, lambsquarters, morningglory spp., pigweed spp., prickly sida, foxtail spp., goosegrass, and others.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.
Corrosiveness: Technical and formulated products are non-corrosive.
Storage stability: Stable over several years; slight sensitivity to natural light and extreme temperatures
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: May cause slight eye, skin, or respiratory tract irritation; if ingested, give 1-2 glasses of water and induce vomiting or lavage stomach; no specific antidote is available, but ingestion of an aqueous slurry of activated charcoal may help inactivate the herbicide
Incompatibilities: Compatible with most other pesticides and fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Symptoms begin with interveinal chlorosis of the leaves and yellowing of leaf margins, followed in susceptible plants by further chlorosis and necrosis. Browning of leaf tips can occur. Root growth is not affected.
Absorption/translocation: Readily absorbed by foliage and roots. Little to no basipetal movement occurs after foliar absorption. Root-absorbed prometon is translocated primarily in the xylem to all parts of the shoot system, with greatest accumulation in mature leaves.
Metabolism in plants: Readily metabolized in tolerant plants by oxidation of the methylthio group to the hydroxy derivative or by conjugation with glutathione. The hydroxy derivative can be further degraded by *N*-dealkylation of the side chains and by hydrolysis of the resulting amino groups on the ring. Both of these metabolism reactions are important for selectivity of most tolerant crop and weed species. Soil placement selectivity is also important for some deep-rooted perennial crops.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Triazine resistance in many weed species is conferred by a single base-pair difference in the *psbA* gene that codes for the D1 protein associated with photosystem II. This change results in the inability of triazine herbicides (including prometryn) to bind to D1. Thus, triazines do not inhibit photosynthetic electron transport in resistant weed biotypes.

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to soil

K_{oc} and K_d: Average K_{oc} is 400 mL/g (2); K_{oc} 247 mL/g and K_d 0.86 mL/g for a sand with 0.6% OM, 1% clay, and pH 7.9; K_{oc} 169 and K_d 1.69 mL/g for a loamy sand with 1.7% OM, 3% clay, and pH 7.7; K_{oc} 117 mL/g and K_d 2.06 mL/g for a silt loam with 3.0% OM, 17% clay, and pH 6.5; K_{oc} 448 mL/g and K_d 3.18 mL/g for a silty clay loam with 1.2% OM, 34% clay, and pH 6.9.

Transformation:

Photodegradation: Stable in water at approximately 18-28 C and pH 7 with natural light, producing hydroxy prometryn [4,6-bis[(1-methylethyl)amino]-1,3,5-triazine-2(1*H*)-one] (2.2% of applied after 30 d); stable on sandy loam soil at 15-28 C with natural light, producing hydroxy prometryn (3.5% after 30 d); negligible contribution to dissipation in the field

Other degradation: Half-life was 261 d for aerobic microbial metabolism in sandy loam soil at 25 C in the laboratory, producing (after 102 d) low levels of hydroxy prometryn, the mono-*N*-dealkylated metabolite [*N*-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine], and the di-*N*-dealkylated metabolite [6-(methylthio)-1,3,5-triazine-2,4-diamine]. Prometryn applied under anaerobic conditions is stable in a sandy loam at 25 C. Aerobic microbial metabolism is the most important contributor to field dissipation. Non-microbial degradation contributes negligibly to field dissipation at pH 5, 7, or 9, producing low levels of hydroxy prometryn as well as the monoamino and diamino metabolites.

Persistence: Average field half-life is 60 d (2)

Field experiments: Half-lives in bareground dissipation studies sampling 0-15 cm: 70 d for silt loam with 2.1% OM and pH 7.7 in Texas; 71 d for sandy loam with 0.9% OM and pH 7.4 in California. Application rate and environmental and edaphic conditions can significantly impact half- life.

Mobility: In field experiments conducted in cotton grown in Texas, no quantifiable prometryn residues (LOD = 10-25 mg/kg) were found below 30 cm

Volatilization: Low volatilization losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade prometryn unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 4550 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat, >5.17 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

CAPAROL 4L: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >2.2 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, mild

CAPAROL 80W: Oral LD_{50} rat, 3920 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >2.35 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL 50 mg/kg; kidney effects in females at 5000 mg/kg

90-d dietary, dog: NOEL 200 mg/kg; slight body weight and liver effects at 2000 mg/kg

21-d dermal, rabbit: NOEL 1000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL 1 mg/kg/d; not carcinogenic; body weight effects at 1000 and 3000 mg/kg

24-mo dietary, rat: NOEL 750 mg/kg; not carcinogenic; body weight and kidney effects at 1500 mg/kg

24-mo dietary, dog: NOEL 4 mg/kg/d; liver and kidney effects at 1500 mg/kg

Teratogenicity:

Rat: NOEL 50 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 12 mg/kg/d, developmental 72 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 10 mg/kg; reduced body weights in dams and offspring at 750 and 1500 mg/kg; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; Mouse lymphoma/L51784/TK+1, negative

Structural chromosome aberration: Human lymphocytes, negative; Chinese hamster/nucleus anomaly, negative

DNA damage/repair: Human fibroblasts, negative; Rat hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck oral LD_{50}, >4640 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Earthworm LC_{50} in soil, 153 mg/kg; Honey bee oral LD_{50}, >130 µg/bee; topical LD_{50}, >99 µg/bee; Daphnia 48-h LC_{50}, 18.9 mg/L; Bluegill sunfish 96-h LC_{50}, 10 mg/L; Rainbow trout 96-h LC_{50}, 2.5 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Successive *N*-alkylation of cyanuric chloride followed by reaction with methylmercaptan to attach the thiomethyl group

Purification of technical: Recrystallization from toluene

Analytical methods: Crop samples are extracted by reflux in 90% methanol. The extract is acidified and partitioned with hexane to remove co-extractives. The aqueous fraction is then made basic and residues are partitioned into dichloromethane. Extracts are analyzed by GC with flame photometric detection in the sulfur-selective mode. Soil samples are extracted with 80% acetonitrile. Residues are partitioned into dichloromethane and analyzed by GC with N/P detection. Water samples are partitioned with dichloromethane, the organic layer is concentrated, and residues are determined by GC with N/P or mass selective detection. Prometryn is determined in technical samples and formulations using GC with flame ionization or flame photometric detection.

Historical: Synthesis and testing of triazine compounds as herbicides began in 1952 in the Geigy Laboratories in Basel, Switzerland. Prometryn was first released for experiment station evaluation in 1959 and became commercially available in 1964 for use in cotton. First reported in 1962 (1). Swiss patent 337,019 and British patent 814,948.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; Agriliance; Gowan; Griffin; Syngenta Crop Protection; UAP-Platte

Reference(s):

1. Gysin, H. 1962. Chem. Ind. (London) p. 1393.
2. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

pronamide

3,5-dichloro-*N*-(1,1-dimethyl-2-propynyl)benzamide

CAS #: 23950-58-5

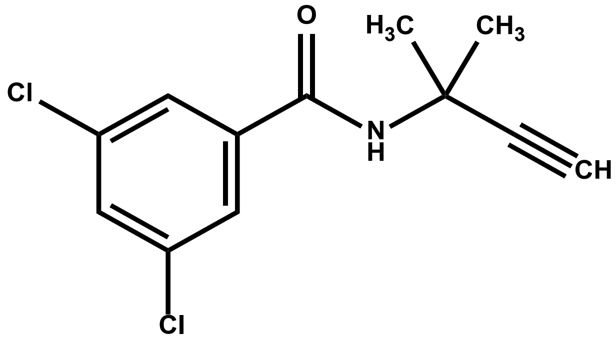
$3^{(K_1)}$

NOMENCLATURE

Common name: pronamide (WSSA)
Other name(s): propyzamide; RH-315; 3,5-dichloro-*N*-(1,1-dimethyl—2-propynyl)benzamide (IUPAC)
Trade name(s): KERB®;
Chemical family: benzamide ; substituted benzamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
pronamide



Molecular formula: $C_{12}H_{11}Cl_2NO$
Molecular weight: 256.13 g/mole
Description: Crystalline powdery solid, very faint musty odor
Density: 1.3441 D^{20}_{4}
Melting point: 155.5-156.5 C
Boiling point: 283 C
Vapor pressure: 5.8×10^{-5} Pa (25 C)
Stability: Thermally stable up to 280 C; stable to hydrolysis in water at pH 4.7-8.8
Solubility:
water 15 mg/L (25 C)
organic solvents g/100 mL (24 C):
acetonitrile 10
chlorobenzene 12
cyclohexanone 20
dimethylformamide 33
isophorone 20
isopropanol 15
mesityl oxide 20
methanol 15
DMSO 33
methyl ethyl ketone 20
ethylene dichloride 5 xylene 10
organic solvents g/100 mL (20 C):
acetone 14
hexane 0.05
ethyl acetate 9
dichloromethane 9
toluene 6

pK_a: None (non-ionizable)
K_{ow}: 1570 (25 C)

HERBICIDAL USE

Pronamide can be applied as follows: PRE at 2.24-4.48 kg ai/ha in artichokes: at 1.12-3.36 kg ai/ha in blackberries, boysenberries, and raspberries at 1.12-2.24 kg ai/ha in blueberries; at 0.21 kg ai/ha in established grasses in the Conservation Reserve Program; at 0.28-0.56 kg ai/ha on fallow: in fall or winter at 0.56-2.24 kg ai/ha in established legumes for forage and seed preplant, PRE, or POST at 1.12-2.24 kg ai/ha in lettuce, endive, and escarole; at 1.12-2.24 kg ai/ha in established rhubarb, woody ornamentals, nursery stock, and Christmas trees; at 1.12-4.48 kg ai/ha in apple, cherry, nectarine, peach, pear, plum, and grape plantings; and early POST at 0.84 kg ai/ha in winter peas. Pronamide has PRE activity against many annual broadleaf and grass weeds including barnyardgrass, carpetweed, large crabgrass, henbit, common lambsquarters, and purslane, and has POST activity against several additional species such as foxtail barley, annual bluegrass, and chickweed.

USE PRECAUTIONS

Fire hazard: KERB 50-W is a dry wettable powder and is non-flammable. Kerb SC is a non-flammable suspension concentrate.
Corrosiveness: KERB 50-W and Kerb SC are non-corrosive.
Storage stability: No storage problems under normal conditions; store dry and cool, but not below 0 C. Storage at >50 C should be avoided. No decomposition or pronamide occurred in a 2-yr storage trial.
Cleaning glassware/spray equipment: Wash with water
Emergency exposure: Hold eye open and rinse slowly and gently with water for 15-20 minutes. Remove contact lenses, if present, after the first 5 minutes, then continue rinsing eye. Call a Poison Control Center or doctor for treatment advice.,

BEHAVIOR IN PLANTS

Mechanism of action: Disrupts cell division by inhibiting mitosis in late prometaphase. (more details on page 12)
Symptomology: Root tips swell.
Absorption/translocation: Readily absorbed into roots and distributed throughout the plant by upward translocation in the apoplast. Pronamide is active when soil-applied and root-absorbed, and has foliar activity on certain weed species. Translocation of leaf-absorbed pronamide is negligible.
Metabolism in plants: Metabolized slowly by both tolerant and sensitive plants. Observed metabolites result from aberrations of the aliphatic side chain (5); producing the ketone and 3,5-dichlorobenzoic acid in lettuce (2).
Non-herbicidal biological properties: Occasionally used by plant breeders as a mitotic inhibitor.
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption:
Koc values in six soils are in the range 548 to 1340 mL/g (average 840 mL/g). Kd values are in range 3.2 to 10.1 mL/g (average 5.8 mL/g).

Transformation:

Photodegradation: Based on lab photolysis half-life of 249 days, very little photolysis losses would occur in field situations.

Other degradation: Pronamide undergoes microbial degradation in aerobic soil to form two major metabolites and carbon dioxide. The half-lives in lab studies were in the range 20 to 392 days (average 120 days).

Persistence: Field half-lives were in the range 18 to 53 days from dissipation studies conducted in California and Wisconsin.

Mobility: Low to moderate mobility. Little leaching occurs in most soils.

Volatilization: Losses are expected to be insignificant under normal use conditions per the product label, but can be significant under hot, dry conditions.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pronamide.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >2.1 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

28-d dietary, mouse: NOEL 15 mg/kg/d; decreased body weight and food consumption, increased liver weights, and liver histopathology at ≥75 mg/kg

90-d dietary, rat: NOEL 12-15 mg/kg/d; decreased body weight gain and food consumption, and increased liver weight at ≥60 mg/kg

Chronic toxicity:

24-mo dietary mouse: NOEL 15 mg/kg/d; hepatic tumors at ≥75 mg/kg

24-mo dietary, rat: NOEL 8-10 mg/kg/d; liver hypertrophy, thyroid adenomas, and testicular Leydig cell adenomas at 43-55 mg/kg

Teratogenicity:

Rat: NOEL ≥160 mg/kg/day; no developmental toxicity at highest dose tested of 160 mg/kg/day

Rabbit: NOEL 5 mg/kg/day; LOEL 80 mg/kg/day

Reproduction:

Rat: NOEL 16-18 mg/kg/d; decreased parental body weight and feed consumption; liver, adrenal, and thyroid hypertrophy: no effects on reproduction at highest dose tested of 120-130 mg/kg/day

Mutagenicity:

Gene mutation: Ames test, negative; Mouse host-mediated bacterial test, negative; *In vitro* Chinese hamster V79 cells, negative; *In vitro* Chinese hamster CHO cells; negative

Structural chromosome aberration: *In vivo* rat cytogenetics, negative; *In vivo* mouse cytogenetics, negative

DNA damage/repair: Bacterial rec-assay, negative; *In vitro* rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck, oral LD_{50}, >14,000 mg/kg; 8-d dietary LC_{50}, >1000 mg/kg; Honey bee, non-toxic; Daphnia 48-h LC_{50}, >5.6 mg/L; Channel catfish 96-h LC_{50}, >200 mg/L; Goldfish 96-h LC_{50}, 350 mg/L; Guppy 96-h LC_{50}, 150 mg/L; Harlequin fish 96-h LC_{50}, 204 mg/L; Rainbow trout 96-h LC_{50}, 72 mg/L; Green algae 96-H LC_{50}, 5.8 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React 3,5-dichlorobenzyl chloride and 3-amino-methylbutyne.

Purification of technical: Recrystallize twice from isopropanol.

Analytical methods: Microgram quantities of pronamide and terminal metabolites are determined by quantitative hydrolysis under reflux conditions in strong acid. The resulting 3,5-dichlorobenzoate is separated and determined by electron capture-GLC.

Historical: Synthesized by Abbott Laboratories and developed by Rohm and Haas Company. Introduced in 1969. U.S. patent 3,534,098.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Dow AgroSciences

Reference(s):

1. Akashi, T. et al. 1968. Plant Cell Physiol. 29:1053.
2. Rauchaud, J. et al. 1987. Weed Sci. 35:469.
3. Vaughn and Lehnen. 1991. Weed Sci. 39:450.

propachlor

CAS #: 1918-16-7 $15^{(K_3)}$

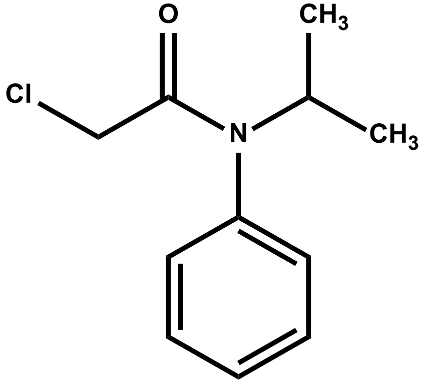
2-chloro-*N*-(1-methylethyl)-*N*-phenylacetamide

NOMENCLATURE

Common name: propachlor (BSI, ISO, WSSA)
Other name(s): propachlore; CP-31393; 2-chloro-*N*-isopropylacetanilide (IUPAC); α-chloro-*N*-isopropylacetanilide (IUPAC)
Trade name(s): RAMROD®; NITACID
Chemical family: acetamide; acetanilide; chloroacetamide; chloroacetanilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
propachlor



Molecular formula: $C_{11}H_{14}ClNO$
Molecular weight: 211.69 g/mole
Description: Light tan solid
Density: 1.13 g/mL (25 C)
Melting point: 77 C
Boiling point: 110 C (4 Pa)
Vapor pressure: 1.05×10^{-2} Pa (25 C)
Stability: Stable to UV light; decomposes at 170 C; Stable at pH 5-9 (25 C)
Solubility:
water 580 mg/L (20 C), 613 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 30.9
benzene 50
carbon tetrachloride 14.8
chloroform 60.2
diethyl ether 21.9
ethanol 29
toluene 34.2
xylene 19.3
pK_a: None (Non-ionizable)
K_{ow}: 201 (25 C)

HERBICIDAL USE

Propachlor can be applied PRE at 2.8-6.7 kg ai/ha in corn, and PRE at 0.67-5.6 kg/ha in grain sorghum. It controls many annual grass weeds such as barnyardgrass, crabgrass spp., foxtail spp., and fall panicum, and certain annual broadleaf weeds such as pigweed spp. and carpetweed.

USE PRECAUTIONS

Fire hazard: All formulated products are dry or aqueous and non-flammable; fire point is 174 C (open cup) for RAMROD 4L.
Corrosiveness: Technical is non-corrosive to #316 and #304 stainless steel, aluminum, and heresite, but is corrosive to ordinary steel.
Storage stability: Dry formulations are stable for at least 4 yr. SC formulations are stable for 1 yr; not sensitive to light
Cleaning glassware/spray equipment: Detergent wash
Emergency exposure: Treat allergic skin reactions as a severe case of poison ivy by a physician. Induce vomiting if ingested.
Incompatibilities: Compatible with water of 1000 mg/L hardness. Compatible with most liquid fertilizers and other pesticides

BEHAVIOR IN PLANTS

Mechanism of action: Site of action is currently thought to be an inhibition of very long chain fatty acid synthesis (VLCFA) (3). Propachlor normally affects susceptible weeds before emergence, but does not inhibit seed germination. (more details on page 14)
Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Injury on corn and sorghum appears as malformed and twisted seedlings. Leaves are tightly rolled in the whorl and may not unroll normally. Injured dicot crops may have cupped or crinkled leaves with a thick, leathery texture. New leaves are puckered with a shortened midrib producing a "drawstring" appearance.
Absorption/translocation: Absorbed primarily by emerging shoots (grass coleoptile, broadleaf hypocotyl or epicotyl). Some root absorption occurs. Plants beyond the seedling stage readily absorb propachlor into the roots and translocate it acropetally throughout the shoots, with primary accumulation in vegetative and less in reproductive parts. Translocation in established plants is irrelevant to mechanism of action because propachlor is phytotoxic only to emerging seedlings. Translocation can occur in both xylem and phloem in established plants.
Metabolism in plants: Metabolized rapidly in plants to metabolites that are similar or identical to those formed in soil.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed, more to OM than to clay. Adsorption increases as OM increases.
K_{oc}: Average is 112 mL/g
K_d: 0.4-1.4 mL/g on four soils with varying properties
Transformation:
Photodegradation: Negligible losses
Other degradation: Propachlor is rapidly degraded under aerobic conditions in all soils. Primary metabolites

are water soluble and involve degradation of the *N*-chloroacetyl group into metabolites containing an oxanilic, oxoacetic, or oxoethanesulfonic acid group.

Persistence: Short persistence with a half-life of 3 d in lab studies with a sandy loam and ~7 d in field studies. Half-life is longer in soils high in OM. Propachlor residues do not injure rotational crops the following season.

Mobility: Propachlor and metabolites are moderately mobile in low OM soils and less mobile in high OM soil. Little movement via runoff is expected.

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade propachlor unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1800 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50} rat, >1.2 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, severe

RAMROD: Oral LD_{50} rat, 3269 mg/kg; Dermal LD_{50} rabbit, 4194 mg/kg; 4-h inhalation LC_{50} rat, 0.69 mg/L; Skin irritation rabbit, severe; Eye irritation rabbit, moderate

RAMROD + ATRAZINE: Oral LD_{50} rat, 2374 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, 9.5 mg/L; Skin irritation rabbit, slight; Eye irritation rabbit, moderate

RAMROD + ATRAZINE DF: Oral LD_{50} rat, 1550 mg/kg; Dermal LD_{50} rabbit, 4550 mg/kg; 4-h inhalation LC_{50} rat, >0.5 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, corrosive

RAMROD 20: Oral LD_{50} rat, 4000 mg/kg; Dermal LD_{50} rabbit, >20,000 mg/kg; 4-h inhalation LC_{50} rat, >4.6 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, yes; Eye irritation rabbit, corrosive

Subchronic toxicity:

90-d dietary, mouse: NOEL NA; decreased body weight gain and food consumption attributed to reduced diet palatibility; liver toxicity

90-d dietary, rat: NOEL NA; decreased body weight gain and food consumption attributed to reduced diet palatibility; reduced spleen weight, anemia, and changes in serum enzymes

90-d dietary, dog: NOEL 45 mg/kg/d; reduced food consumption and body weight attributed to reduced diet palatability

Chronic toxicity:

18-mo dietary, mouse: NOEL 1.6 mg/kg/d; liver and kidney organ weight changes; not oncogenic

24-mo dietary, rat: NOEL 2.6 mg/kg/d; liver toxicity; not oncogenic

12-mo dietary, dog: NOEL 9 mg/kg/d; decreased weight gain attributed to reduced diet palatability

Teratogenicity: No birth defects at dosages producing mild toxicity in the offspring

Rat: NOEL 200 mg/kg/d; not teratogenic

Rabbit: NOEL 58 mg/kg/d; not teratogenic

Reproduction: No reproductive effects at dosages producing mild toxicity in the offspring.

Rat: NOEL 30 mg/kg/d

Mutagenicity: Propachlor is not considered mutagenic based on evidence from a number of genetic tests. A positive response was reported in only one assay and a weak response in one other

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: CHO/cytogenetics, positive; *In vivo* rat bone marrow, negative; *In vivo* mouse bone marrow, negative

DNA damage/repair: *In vivo* rat hepatocytes, negative; *In vitro* rat hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, 91 mg/kg, 5-d dietary LC_{50}, >5620 mg/kg; Mallard duck 5-d dietary LC_{50}, >5620 mg/kg; Honey bee oral LD_{50}, >1000 mg/kg, topical LD_{50}, >25 μg/bee; Daphnia 48-h LC_{50}, 7.8 mg/L; Bluegill sunfish 96-h LC_{50}, >1.4 mg/L; Rainbow trout 96-h LC_{50}, 0.17 mg/L

RAMROD: Honey bee oral LD_{50}, >1000 mg/kg, topical LD_{50} , >25 μg/bee; Daphnia 48-h LC_{50}, 13 mg/L; Bluegill sunfish 96-h LC_{50}, 1.6 mg/L; Rainbow trout 96-h LC_{50}, 0.42 mg/L

RAMROD + ATRAZINE: Daphnia 48-h EC_{50}, 14 mg/L; Bluegill sunfish 96-h LC_{50}, 2.5 mg/L; Rainbow trout 96-h LC_{50}, 0.75 mg/L

Use classification: General Use for formulated products containing propachlor only. RAMROD + ATRAZINE formulations are Restricted Use because of groundwater contamination concerns with atrazine.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React *N*-isopropyl aniline with chloroacetylchloride

Purification of technical: Crystallization

Analytical methods: See FDA Pesticide Analytical Manual, Vol. II, section 180.211

Historical: Herbicidal activity of the chloroacetamides was discovered in 1952 by Monsanto (2). U.S. patent 2,863,752 was issued to Monsanto. Propachlor was developed in the early 1960s and commercially introduced as RAMROD in 1965 by Monsanto.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Monsanto

Reference(s):

1. Fuerst, E. P. 1987. Weed Technol. 1:270.
2. Hamm, P. C. 1974. Weed Sci. 22:541.
3. Böger P., Matthes, B., and Schmalfuss, J. 2000. Pest. Manag. Sci. 56:497-508.

propanil

N-(3,4-dichlorophenyl)propanamide

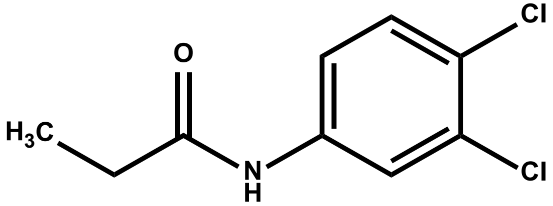
CAS #: 709-98-8 $7^{(C_2)}$

NOMENCLATURE

Common name: propanil (BSI, ISO, WSSA)
Other name(s): BAY 30130; DCPA (JMAF); DCP; DPA; ERBAN; FW-734; PROPANILE; PROPANILO; PROPANOL; S-10145; S-10165; *N*-(3,4-dichlorophenyl) propionamide; 3′,4′-dichloropropionanilide (IUPAC)
Trade name(s): BLUE DRUM PROPANIL; PROSTAR; CEKUPROPANIL; CHEM-RICE; PROPANEX®; ROGUE; SUPERWHAM!™; STAM®; STAMPEDE®; STREL®; SURCOPUR; VERTAC; WHAM!
Chemical family: amide; acetamide; substituted amide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
propanil



Molecular formula: $C_9H_9Cl_2NO$
Molecular weight: 218.08 g/mole
Description: Brown to black crystalline solid (colorless when pure), organic acid odor
Density: ~1.25 g/mL (25 C)
Melting point: 85-89 C (technical); 92-93 C (pure)
Boiling point: >400 C
Vapor pressure: 5×10^{-3} Pa (20 C); 1.2×10^{-2} Pa (60 C)
Stability: Hydrolyzes to 3,4-dichloroaniline and propionic acid under strong acid or alkaline conditions
Solubility:
water 500 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 170
benzene 7
cyclohexanone 35
ethanol 110
hexalene glycol >25
isophorone 52
isopropanol >25
mesityl oxide 50
methyl ethyl ketone 25
toluene >25
xylene >25
pK_a: None (non-ionizable)
K_{ow}: 193 (20 C)

HERBICIDAL USE

Propanil can be applied POST at 3.6-5.6 kg ai/ha in rice, and POST at 1.08-1.28 kg ai/ha in wheat and barley. It controls certain annual broadleaf and grass weeds such as foxtail spp. and pigweed spp. At the higher rates used in rice, propanil controls additional species including barnyardgrass, crabgrass spp., woolly croton, goosegrass, and Mexican weed.

USE PRECAUTIONS

Fire hazard: Propanil technical is nonflammable; flash point is >100 C. STAM M4, STAM 4E, and STREL 4E are non-flammable; flash points are 43 C (Seta closed cup). WHAM! EZ is aqueous and nonflammable. PROPANIL 4 and PROPANEX 4 are marginally flammable; flash points are 38 C (TCC). WHAM! DF 80, STAM 80 EDF, and STAMPEDE 80 EDF are dry and non-flammable.
Corrosiveness: All formulated products corrode steel. Dry formulations are less corrosive than ECs.
Storage stability: Do not store STAM M-4, STAM 4E, or STREL below 0 C, and STAMPEDE below -9.4 C. Shelf life of WHAM! DF 80 is indefinite if protected against moisture. Shelf life of WHAM! EZ is ~2 yr. STAM 80EDF has indefinite shelf life if kept dry.
Cleaning glassware/spray equipment: Wash with water or isopropanol.
Emergency exposure: Wash skin with soap and water; may cause irritation. Flush eyes for at least 15 min and get medical attention. If ingested, induce vomiting or administer gastric lavage; when vomit fluid is clear, give as much milk as the patient can tolerate. Sodium or magnesium sulfate may be given as a saline laxative. Symptoms of poisoning include local irritation and central nervous system depression or, if ingested, gagging, coughing, nausea, and vomiting followed by headache, dizziness, drowsiness, and confusion.
Incompatibilities: Tank-mix application with other herbicides, insecticides, spray adjuvants, or liquid fertilizers may reduce crop tolerance and weed control or impair mixing properties. Propanil tank mixed with carbamate and organophosphorus insecticides often causes crop injury.

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood; may inhibit photsystem II electron transport. Other reported effects include inhibition of anthocyanin sythesis, RNA and proteins as well as adverse effects on the plasmalemma (1). (more details on page 13)
Symptomology: Chlorosis begins within a few to several days, followed by foliar desiccation and necrosis.
Absorption/translocation: Readily absorbed by foliage. Limited movement from treated leaf to growing point, and then back to other leaves (8). Maximum efficacy requires a rain-free period of 4-8 h after application.
Metabolism in plants: Rapidly hydrolyzed in rice by an aryl acylamidase to 3,4-dichloroaniline (2, 9). Propanil tolerance in rice and wheat is attributed to higher acylamidase activity in these crops compared to activity found in susceptible weeds such as barnyardgrass (5).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Propanil-resistant *Echinochloa colonum* and *E. crus-galli* were found in Colombia and Greece, respectively (3). Propanil-resistant

E. colonum also has been documented in Arkansas (6).

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil

K_{oc} and K_d: Weakly adsorbed to soil. Average K_{oc} is 149 mL/g (7). K_{oc} 306 mL/g and K_d 0.54 mL/g for a sand with 0.3% OM; K_{oc} 239 mL/g and K_d 2.32 mL/g for a sandy loam with 1.65% OM; K_{oc} 800 mL/g and K_d 8.00 mL/g for a silt loam with 1.7% OM; K_{oc} 398 mL/g and K_d 11.7 mL/g for a clay loam with 5.0% OM

Transformation:

Photodegradation: Half-life in water was 102.5 d for irradiated samples (714.4 d for dark samples). In water, a ring Cl may be lost together with urea hydrolysis to produce 3-chloroaniline and 3,4-dichloroaniline.

Other degradation: Rapidly metabolized to propionic acid and 3,4-dichloroaniline (DCA) in aerobic rice paddy water, followed (7 d after application) by DCA degradation to volatiles and residues strongly bound to sediment. Metabolism in anaerobic paddy water was similar except that DCA degradation occurred 14 d after application. Most DCA becomes covalently bound to soil OM and degrades very slowly (half-life of several years). Some DCA is converted by microbial peroxidases to 3,4-dichlorophenylhydroxylamine which condenses with DCA to form 3,3′,4,4′-tetrachlorohydrazobenzene, followed by oxidation to 3,3′,4,4′-tetrachloroazobenzene (4).

Persistence: Typical field half-life is 1 d (7), but ranges from 1-3 d under warm, moist conditions. Residues do not injure crops planted the following season.

Lab experiments: Half-life was 2 d in aerobic rice paddy water, and 2-3 d in anaerobic paddy water.

Mobility: Moderate mobility in sand and low mobility in soils with higher clay content. Leaching to groundwater is highly unlikely given rapid propanil degradation in soil.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade propanil unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 1080 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, 1.12 mg/L; Skin irritation, NA; Skin sensitization guinea pig, no; Eye irritation rabbit, yes

PROPANIL 4: Oral LD_{50} rat, 1870 mg/kg; Dermal LD_{50} rabbit, <2000 mg/kg; Skin irritation rabbit, slight; Eye irritation rabbit, mild-strong

WHAM DF 50: Oral LD_{50} rat, >1000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild-strong

WHAM! EZ: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild-strong

STAM 80 EDF: Oral LD_{50} rat, >500 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50}, >6.06 mg/L; Skin irritation rabbit, slight; Eye irritation rabbit, moderate

STAM M-4: Oral LD_{50} rat, >500 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50}, >2.8 mg/L; Skin irritation rabbit, moderate; Eye irritation rabbit, substantial

Subchronic toxicity:

90-d dietary, mouse: NOEL 5 mg/kg/d; liver and blood effects, and cyanosis at ≥25 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL NA; not carcinogenic

24-mo dietary, rat: NOEL NA; not carcinogenic

12-mo dietary, dog: NOEL 400 mg/kg decreased weight gain at 4000 mg/kg; feed consumption increased, but feed efficiency decreased with time

Teratogenicity:

Rat and rabbit: NOEL 20 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 300 mg/kg; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative with or without metabolic activation; CHO/HGPRT, negative; CHO, negative

Structural chromosome aberration: *In vivo* mouse cytogenetics, negative

DNA damage/repair: Rat hepatocytes, negative

Wildlife:

Bobwhite quail oral LD_{50}, 196 mg/kg; 8-d dietary LC_{50}, 2861 mg/kg; Mallard duck 8-d dietary LC_{50}, 5627 mg/kg; Daphnia 48-h EC_{50}, 0.14 mg/L, NOEC 0.086 mg/L; Bluegill sunfish 96-h LC_{50}, 5.4 mg/L; Sheepshead minnow 96-h LC_{50}, 4.6 mg/L; Rainbow trout 96-h LC_{50}, 2.3 mg/L; Eastern oyster 96-h LC_{50}, 5.8 mg/L; 96-h NOEC, 1.4 mg/L; Mysid shrimp 96-h LC_{50}, 0.4 mg/L, 96-h NOEC, 0.18 mg/L

PROPANIL 4: Daphnia 48-h LC_{50}, 1.2 mg/L; 48-h NOEC, 0.59 mg/L; Bluegill sunfish 96-h LC_{50}, 14 mg/L, 48-h NOEC, 4.4 mg/L; Rainbow trout 96-h LC_{50}, 13 mg/L, 96-h NOEC, 3.8 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React propionic acid and 3,4-dichloroaniline to form *N*-(3,4-dichlorophynyl) propanamide. Residual 3,4-dichloroaniline is reacted with propionic anhydride. Water and residual propionic acid are vacuum distilled.

Purification of technical: Recrystallization

Analytical methods: Propanil and principal impurities in technical (98%) can be determined by GC with hydrogen flame ionization detection. Alternatively, propanil can be hydrolyzed and reacted with *N*-(1-naphthyl)ethylenediamine to form a brilliant magenta dye which absorbs at 555 nm. See Analytical Methods and Procedures for Plant Growth Regulators and Food Additives, Vol. 4, Herbicides, Academic Press (1964). For residues in plant tissue, see pages 692-696 in Analytical Methods for Pesticides and Plant Growth Regulators, Vol. 6 (1972). For residues in soil, see Bull. Environ. Contam. Toxicol. 29:243 (1982).

Historical: Introduced by Rohm and Haas Company, and later by Bayer CropScience AG and by Monsanto Chemical Company. British patent 93,766 was issued to

Bayer CropScience AG. Propanil was first registered on rice in the U.S. in 1961.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

Reference(s):

1. Devine, M., S. O. Duke, and C. Fedtke. 1993. Physiology of Herbicide Action. Prentice Hall, New Jersey.
2. Hirase and Matsunaka. 1991. Pestic. Biochem. Physiol. 41:82.
3. LeBaron, H. M. 1991. Pages 27-66 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Ltd., Oxford.
4. Pothuluri, J. V. et al. 1991. J. Environ. Qual. 20:330.
5. Shimabukuro, R. H. 1985. Pages 215-240 *in* S. O. Duke, ed., Weed Physiology, Vol. II Herbicide Physiology. CRC Press, Inc., Boca Raton, FL.
6. Smith and Baltazar. 1992. Abstr. Weed Sci. Soc. Am. 32:21.
7. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
8. Yamada and Nakamura. 1963. Proc. Crop Sci. Soc. Japan 32:69.
9. Yih, R. Y. et al. 1968. Science 161:376.

propaquizafop

CAS #: 111479-05-1

$1^{(A)}$

2-[[(1-methylethylidene)amino]oxy]ethyl (2R)-2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]propanoate

NOMENCLATURE

Common name: propaquizafop (R-isomer) (ISO)

Other name(s): 2-isopropylideneaminooxyethyl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy] propionate

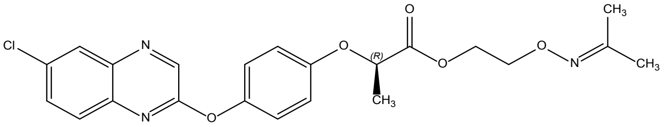
Trade name(s): CORRECT®; SHOGUN®; AGIL®

Chemical family: aryloxyphenoxy propionate; aryloxyphenoxy propionic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

propaquizafop



Molecular formula: $C_{22}H_{22}ClN_3O_5$

Molecular weight: 443.89 g/mole

Description: Clear yellow liquid

Density: 1.3 g/mL

Melting point: 66.3 C

Boiling point: NA

Vapor pressure: 4.4×10^{-7} Pa (25 C)

Stability: >2 yr in closed container at room tempera-ture; moderately stable at acid and neutral pH. ; rapidly hydrolyzed under alkaline conditions; stable to ultraviolet light

Solubility: (25 C) 0.63 mg/L in water, 59 mg/L in ethanol, 730 mg/L in acetone, 630 mg/L in toluene, 37 mg/L in n-hexane, 16 mg/L in n-octanol

pK$_a$: None (non-ionizable)

K$_{ow}$: log K_{ow} = 4.78 (25 C)

HERBICIDAL USE

Propaquizafop is used for control of a wide range of annual and perennial grasses (including Sorghum halepense, Elytrigia repens, and Cynodon dactylon) in soybean, cotton, sugar beet, potatoes, peanut, peas, oilseed rape, and vegetables.

USE PRECAUTIONS

Fire hazard: Non-flammable; Liquid formulations containing organic solvents may be flammable.

Corrosiveness: Non-corrosive

Storage stability: Stable

Emergency exposure: Swallowing: Do not induce vomiting. Give glass of milk and seek medical attention.

Eye Exposure: Flush with large quantities of water for at least 15 min. Seek medical attention.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details of page 12)

Symptomology: Treated grasses cease growth within 3-4 d, show chlorosis of younger plant tissues, followed by a progressive collapse of the entire plant 10-20 d later.

Absorption/translocation: Absorbed by foliage and roots and translocated throughout the plan predominately in the phloem

Metabolism in plants: Rapidly metabolized in soybean, sugar beet and cotton foliage to the free acid, followed by further metabolism to the quinoxaline oxyphenol

Mechanism of resistance in plants: Weed biotypes resistant to other ACCase inhibitors are resistant to propaquizafop

BEHAVIOR IN SOIL

Sorption:

K$_{oc}$: 204-472 mL/g

Transformation:

Photodegradation: NA

Other degradation: NA

Persistence: Field dissipation DT_{50} = 3 d

Mobility: NA

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Acute toxicity:

Oral LD_{50} (rat) >, 5000 mg/kg; mice, 3009 mg/kg; Dermal LD_{50}, > 2000 mg/kg; Inhalation LC_{50} (4 h), 2.5 mg/L air

Chronic toxicity: (2 yr) NOEL for rats and mice 1.5 mg/kg/d, dogs 20 mg/kg/d

Teratogenicity: Non-teratogenic

Reproduction: No reproductive effects observed

Mutagenicity: Non-mutagenic

Wildlife:

Oral LD_{50} Bobwhite quail, > 6593 mg/kg; LC_{50} bluegill sunfish, 3.34 mg/L (96 h); LC_{50} rainbow trout, 1.2 mg/L (96 h); EC_{50} Daphnia magna, > 2 mg/L (48 h); EC_{50} green algae, >2.1 mg/L

Use classification: WHO (a.i.)

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

propoxycarbazone-sodium

CAS #: 181274-15-7 **$2^{(B)}$**

methyl 2-[[[(4,5-dihydro-4-methyl-5-oxo-3-propoxy-1*H*-1,2,4-triazol-1-yl)carbonyl]amino]sulfonyl] benzoate, sodium salt

NOMENCLATURE

Common name: propoxycarbazone-sodium (ISO 1750 provisional)

Other name(s): BAY MKH 6561; sodium 4,5-dihydro-*N*-{[2-(methoxycarbonyl)phenyl]sulfonyl}-4-methyl-5-oxo-3-propoxy-1*H*-1,2,4-triazole-1carboximidate (IUPAC)

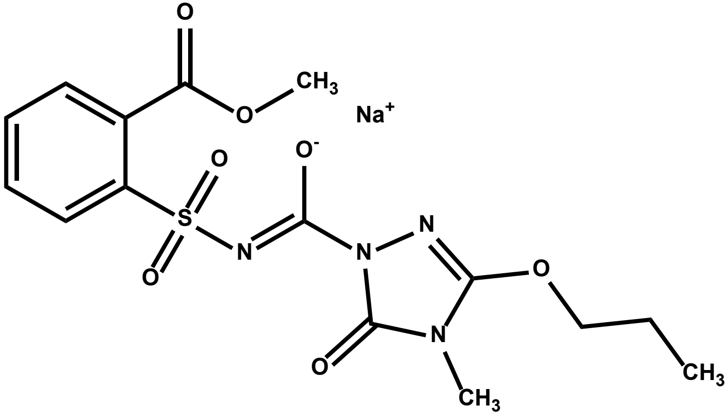
Trade name(s): OLYMPUS®; RIMFIRE™

Chemical family: sulfonylaminocarbonyltriazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

propoxycarbazone-sodium



Molecular formula: $C_{15}H_{17}N_4NaO_7S$

Molecular weight: 420.37 g/mole

Description: Colorless crystalline powder

Density: NA

Melting point: 230-240 C

Boiling point: 129 C (4.40 x 10^3 Pa)

Vapor pressure: <1.0 x 10^{-8} Pa (20 C)

Stability: stable (pH 4-9)

Solubility: (20 C)
(pH 4) 2900 mg/L
(pH 7) 42,000 mg/L
(pH 9) 42,000 mg/L

pK_a: 2.1 (weak acid)

K_{ow}: log K_{ow} = -0.3 (pH 4); -1.55 (pH 7); -1.59 (pH 9)

HERBICIDAL USE

Propoxycarbazone-sodium provides activity against grass weeds and several important broadleaf weeds when applied POST to wheat. It has demonstrated activity against *Alopecurus myosuroides, Bromus spp.* and *Elymus repens.* Use rate is 42 - 70 g a.i./ha.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: NA

Storage stability: NA

Cleaning glassware/spray equipment: NA

Emergency exposure: NA

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Weeds cease to grow and compete with crop soon after application. Further symptoms will develop over 1-4 wk depending on environmental conditions and include stunting, discoloration and necrosis.

Absorption/translocation: Propoxycarbazone is absorbed through the foliage and root system. Acropetal and basipetal translocation occurs in treated plants.

Metabolism in plants: NA

Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption:

Transformation:

Photodegradation: Propoxycarbazone has an aqueous photolytic half-life of 30 d in pure water and 36 d in soil.

Other degradation: The primary route of degradation is believed to be microbial.

Persistence:

Field experiments: $t_{1/2}$ = 9 d

Volatilization: Minimal

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade propoxycarbazone-sodium unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, > 5000 mg/kg; Dermal LD_{50} rat, >5000 m^3 (non-irritating); Dermal inhalation LC_{50}, >5030 mg/m^3

Chronic toxicity:

In chronic studies, no evidence for neurotoxic, genotoxic, carcinogenic potential nor teratogenic or reproductive toxicity

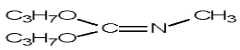
Wildlife:

Bobwhite quail acute oral LD_{50}, >2000 mg/kg; subacute dietary LC_{50}, >5000 mg/kg; aquatic organisms (LC_{50}); Bluegill sunfish, >94.7 mg/L (96 h); Rainbow trout, >77.6 mg/L (96 h); Daphnia, >107 mg/L; Green algae, 1.57 mg/L; Earthworm LC_{50}, >1000 mg/kg soil; Honeybee oral LD_{50}, >319 µg/bee; Contact LD_{50}, >200 µg/bee

Use classification: EPA Category IV

SYNTHESIS AND ANALYTICAL METHODS

Phenyl hydrazinecarboxylate +


$(C_3H_7O)_2C{=}N{-}CH_3$

in the presence of 1,2-dichlorobenzene creates 4-methyl-3-propoxy-1,2,4-triazin-5-one which is combined with 2-carbomethoxyphenyl-sulfonyl isocyanate to yield propoxycarbazone.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1. Feucht, D., K. H. Müller, and A. Wellman. 1999. Proc. Br. Crop Prot. Conf. – Weeds, Vol. 1:53-58.

prosulfocarb

CAS #: 52888-80-9 **$8^{(N)}$**

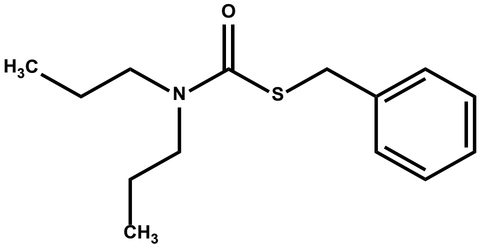
S-(phenylmethyl)dipropylcarbamothioate

NOMENCLATURE

Common name: prosulfocarb (BSI, draft E-ISO)
Other name(s): ICI-A0574; *S*-benzyl dipropyl(thiocarbamate) (IUPAC)
Trade name(s): BOXER; DEFI
Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
Prosulfocarb



Molecular formula: $C_{14}H_{21}NOS$
Molecular weight: 251.39 g/mole
Description: Colorless liquid
Density: 1.04 g/mL
Melting point: NA
Boiling point: 129 C (4.40 x 10^3 Pa)
Vapor pressure: 6.9 x 10^{-3} Pa (25 C)
Stability: Stable for at least 2 mo at 52 C
Solubility:
water 13.2 mg/L (20 C)
miscible with acetone, chlorobenzene, ethanol, xylene, ethyl acetate, kerosene
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 4.65 (25 C)

HERBICIDAL USE

Pre and early post control of wide range of grass and broadleaf weeds in winter wheat, winter barley and rye, at 3-4 kg ai/ha. Controls *Galium aparine*, but also *Alopecurus myosuroides, Poa annua, Stellaria media, Sinapis arvensis, Veronica spp. and Lolium multiflorum*.

USE PRECAUTIONS

Fire hazard: Keep fire exposed containers cool by spraying with water; non-explosive. Flash point is 132 C. Combustion/ thermal decomposition will evolve toxic and irritant vapors.
Storage stability: Stable at room temperature; store above –10C
Emergency exposure: If ingested, do not induce vomiting. Seek medical advice. On eye contact, irrigate eyes for at least 15 min with water.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)
Symptomology: Dark greening, twisting, inhibition of shoots and roots and failure of leaf emergence from coleoptiles
Absorption/translocation: Absorbed by leaves and roots
Metabolism in plants: NA
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: None known

BEHAVIOR IN SOIL

Sorption: K_{oc} ranges from 1367 to 2340 mL/g (5)
Transformation:
Photodegradation: NA
Other degradation: Microbial, half-life is 12-49 d at 21.5 C, aerobic. It is substantially biodegradable in water and soil.
Persistence: 81% degraded after 28 d
Mobility: NA
Volatilization: Low volatility

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade prosulfocarb unless otherwise indicated.

Acute toxicity:
Oral LD_{50} for male rats, 1820, female rats, 1958 mg/kg; Dermal LD_{50} for rabbits, >2000mg/kg; LC_{50} (4h) inhalation rat, >4.7mg/L; Skin irritation rabbit, mild; Eye irritation rabbit, mild; Skin sensitization guinea pigs, none
Chronic toxicity:
Repeated doses produce no significant effects **Teratogenicity:**
Rat: Non-teratogenic
Rabbit: Non-teratogenic
Reproduction: NA
Mutagenicity:
Gene mutation: Non-mutagenic in the Ames test Structural chromosome aberration:
Wildlife:
Bobwhite quail LD_{50}, >2250 mg/kg; LC_{50} for Mallard duck, >5620 mg/kg; LC_{50} (96 h) for bluegill sunfish, 4.2 mg/L; rainbow trout, 1.7 mg/L; Daphnia EC_{50} (48 h), 1.3 mg/L; bees LD_{50} (48 h) contact, >79 mg/bee, oral 103 mg/bee
Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: Discovered by Stauffer Chemical and introduced in Belgium in 1988.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Casida, J. E. et al. 1974. Science 184:573.
2. Fuerst, E. P. 1987. Weed Technol. 1:270-277.
3. Gronwald, J. W. 1991. Weed Sci. 39:435.
4. Prakash, T. R. et al. 1989. Weed Res. 19:427

prosulfuron

CAS #: 94125-34-5 **2$^{(B)}$**

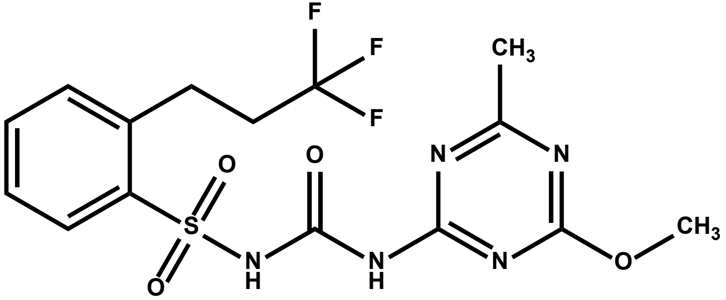
1-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)-3-[2-(3,3,3-trifluoropropyl)phenylsulfonyl]urea

NOMENCLATURE

Common name: prosulfuron (ISO)
Other name(s): CGA-152005; 1-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)-3-[2-(3,3,3-trifluoropropyl)phenylsulfonyl] urea (IUPAC)
Trade name(s): BRONS; ECLAT; EXCEED™; PEAK®; SPIRIT® CASPER®
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
prosulfuron



Molecular formula: $C_{15}H_{16}F_3N_5O_4S$
Molecular weight: 419.38 g/mole
Description: Colorless crystalline solid, odorless
Density: 1.45 g/mL
Melting point: 165.2 C (with decomposition)
Boiling point: NA
Vapor pressure: $<3.46 \times 10^{-6}$ Pa (25 C)
Stability: Stable at room temperature
Solubility:
water 30 mg/L (pH 5.1, 20 C); (pH 6.8, 20 C) 3580 mg/L
organic solvents g/100 mL (25 C):
acetone 16 *n*-hexane 0.0003
ethanol 1 methanol 2.1
pK$_a$: 3.76 (weak acid)
K$_{ow}$: 33.98 (pH 5); 0.6138 (pH 6.9); 0.1757 (pH 9)

HERBICIDAL USE

Prosulfuron can be applied POST at 15-40 g ai/ha in corn, grain sorghum, wheat, barley, sugarcane, and certain other graminaceous crops. It controls certain annual broadleaf weeds such as cocklebur, kochia, lambsquarters, pigweed spp., ragweed spp., and velvetleaf. A surfactant or oil adjuvant is required for maximum POST efficacy. Prosulfuron provides residual weed control in addition to POST activity.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Formulated products are non-corrosive.
Storage stability: Good stability; formulated products may be stored as low as -34 C.
Cleaning glassware/spray equipment: Clean glassware and equipment with 2% v/v ammonia; use a pressure rinser to direct the ammonia solution inside the tank; clean nozzles and screens separately.
Emergency exposure: If ingested, drink 1-2 glasses of water and induce vomiting. If large amounts have been ingested and emesis is inadequate, lavage stomach and treat symptomatically. No specific antidote is available. Slight temporary eye or skin irritation can occur.
Incompatibilities: Certain organophosphate insecticides (especially terbufos) applied at planting or tank mixed with prosulfuron may facilitate prosulfuron injury on corn. POST application of an organophosphate insecticide within 10 d before or 5 d after prosulfuron application may result in crop injury. Prosulfuron applied in liquid fertilizer carrier may result in crop injury.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth is rapidly inhibited in susceptible species, resulting in stunted plants. Foliar chlorosis appears within 5-7 d, followed by chlorosis and necrosis of the growing point of broadleaf plants, and general foliar necrosis. Complete plant death may require 14-21 d.
Absorption/translocation: Readily absorbed by foliage and roots, with extensive translocation in both xylem and phloem; foliar-applied prosulfuron translocates to the shoot meristems and at moderate levels to roots; root-absorbed prosulfuron translocates to all parts of the shoots
Metabolism in plants: Rapidly metabolized in corn by hydroxylation of the phenyl ring to produce the 5-hydroxy metabolite. Hydrolytic cleavage of the sulfonylurea bridge before or after phenyl hydroxylation yields additional metabolites including the trifluoropropyl benzene sulfonamide, its 5-hydroxy analog, the triazine moiety of the parent herbicide and its *O*-demethylated analog. The 5-hydroxy phenyl derivatives are conjugated to sugars to produce water-soluble metabolites. The unmetabolized parent herbicide was not detectable in corn 30 d after application.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Sulfonylurea-resistant weed biotypes selected in the field by chlorsulfuron use typically are resistant to prosulfuron. The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme. An alternative resistance mechanism involves enhanced sulfonylurea herbicide degradation by cytochrome P450 enzymes. Biotypes with this latter mechanism may be cross-resistant to herbicides from several chemical families.

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil

K_{oc} and K_d: K_{oc} 17.6 mL/g and K_d 0.07 mL/g for a loamy sand with 0.8% OM, 8% clay, and pH 7.7; K_{oc} 15.25 mL/g and K_d 0.27 mL/g for a sandy loam with 3.4% OM, 19% clay, and pH 7.8; K_{oc} 18.56 mL/g and K_d 0.29 mL/g for a silt loam with 3% OM, 17% clay, and pH 6.5; K_{oc} 41.3 mL/g and K_d 0.25 mL/g for a silty clay loam with 1.16% OM, 34% clay, and pH 6.9

Transformation:

Photodegradation: Stable in water at pH 9 and 25 C under sunlight, with a half-life of 157-198 d; photolysis half-life on soil at 25 C under sunlight ranged from 110-131 d

Other degradation: In two different sandy loams, pH values of 6.1 and 6.6, half-lives averaged 118 d and ranged from 70-152 d. Half-life for non-microbial hydrolysis was 10 d at pH 5, but prosulfuron was stable at pH 7 and 9. Non-microbial hydrolysis is a major contributor to field dissipation in acid soils.

Persistence: Moderately persistent. Environmental and edaphic factors (especially pH) can significantly affect half-life.

Field experiments: Half-lives in Georgia were 8.9 d in a corn study and 10.2 d on bare ground; respective half-lives in Iowa were 19.2 and 10.2 d

Mobility: Potentially mobile; in field studies, however, no residues of prosulfuron and three metabolites have been detected below 30 cm

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade prosulfuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 986 mg/kg; Dermal LD_{50} rabbit >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.4 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Prosulfuron 57% WG: Oral LD_{50} male rat, >5050 mg/kg, female rat ,4360 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, mouse: NOEL male 2.01 mg/kg/d, female 91.3 mg/kg/d; decreased body weight gain at 7000 mg/kg; liver, heart, and hematopoietic system were the target organs

90-d dietary, rat: NOEL male 3.1 mg/kg/d, female 35 mg/kg/d; decreased body weight and weight gain in males at ≥500 mg/kg and in females at ≥4000 mg/kg; liver effects in females at 8000 mg/kg

90-d dietary, dog: NOEL male 5.3 mg/kg/d, female 6.5 mg/kg/d; decreased body weight gain at ≥1500 mg/kg; liver and hematopoietic system were target organs at ≥1500 mg/kg, and the heart was a target organ at 3000 mg/kg

21-d dermal, rabbit: NOEL 1000 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL male 1.71 mg/kg/d, female 100 mg/kg/d; not oncogenic at 7000 mg/kg; reduced body weight gain at 7000 mg/kg; hematologic effects in males at >3500 mg/kg and in females at 7000 mg/kg; liver changes in males at >700 mg/kg and in females at ≥3500 mg/kg

24-mo dietary, rat: NOEL 200 mg/kg; reduced body weight and weight gain and slight reductions in hematologic parameters at ≥2000 mg/kg; evidence of an earlier onset of mammary gland tumors at ≥2000 mg/kg (not statistically significant)

12-mo dietary, dog: NOEL male 1.95 mg/kg/d, female 1.84 mg/kg/d; reduced body weight and weight gain at 1200 mg/kg; hematopoietic effects in males at 1200 mg/kg and in females at ≥600 mg/kg; liver changes in both sexes and kidney effects in males at >600 mg/kg

Teratogenicity:

Rat: NOEL 200 mg/kg/d; not teratogenic; maternal toxicity (reduced body weight gain) and increased incidence of skeletal variations in fetuses at 400 mg/kg/d

Rabbit: NOEL 10 mg/kg/d; not teratogenic; maternal toxicity (reduced body weight gain) at 100 mg/kg/d

Reproduction:

Rat: NOEL 13 mg/kg/d in a 2-generation study; not a reproductive toxin at up to 4000 mg/kg; reduced body weight, weight gain, and food consumption at ≥2000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; Chinese hamster V79 cells, negative

Structural chromosome aberration: CHO, negative; Mouse bone marrow/micronucleus test, negative

DNA damage/repair: Rat hepatocytes/autoradiographic DNA repair, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >1094 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Earthworm LC_{50} in soil, >110 mg/kg; Honey bee oral LD_{50}, >100 µg/bee, topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >120 mg/L; Bluegill sunfish 96-h LC_{50}, >155 mg/L; Rainbow trout 96-h LC_{50}, >160 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: A multi-step synthesis begins with aniline-2-sulfonic acid and ending in condensation with the appropriate triazine.

Purification of technical: NA

Analytical methods: Plant material and soil are homogenized with acetonitrile/water, and water samples are extracted with C-18 SPE. Extracts are cleaned-up using liquid-liquid partitioning. Prosulfuron residues are determined with reverse phase HPLC using acetonitrile and a phosphate buffer. LC-MS also has been used for soil and water analysis.

Historical: Prosulfuron was synthesized by Ciba-Geigy Ltd in Basel, Switzerland. It was first field tested in 1988, and in 1994 was tested under an Experimental Use Permit.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. LaRossa and Schloss. 1984. J. Biol. Chem. 259:8753

pyraflufen-ethyl

CAS #: 129630-19-9

14$^{(E)}$

ethyl[2-chloro-5-[4-chloro-5-difluoromethoxy)-1-methyl-1*H*-pyrazol-3-yl]-4-fluorophenoxy]acetate

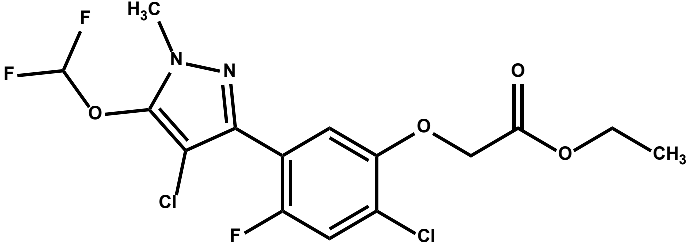
NOMENCLATURE

Common name: pyraflufen-ethyl (ISO)
Other name(s): ET-751; ethyl 2-chloro-5-(4-chloro-5-difluoromethoxy-1-methylpyrazol-3-yl)-4-fluorophenoxyacetate (IUPAC)
Trade name(s): MILAN®; ECOPART
Chemical family: pyrazole; phenylpyrazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

pyraflufen-ethyl



Molecular formula: $C_{15}H_{13}Cl_2F_3N_2O_4$
Molecular weight: 413.18 g/mole
Description: Pale brown crystalline powder
Density: NA
Melting point: 126-127 C
Boiling point: NA
Vapor pressure: 4.79 x 10^{-3} Pa (25 C)
Stability: NA
Solubility: In water, <1 mg/L (25 C); xylene 2.9 mg/L, acetone 25 mg/L; ethanol 1 mg/L; ethyl acetate 14.5 (% w/w)
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 3.49

HERBICIDAL USE

Pyraflufen-ethyl provides selective postemergence control of broadleaf weeds including *Galium aparine*, *Marticaria inodora*, *Laminum purpureum*, and *Stellaria media* in cereals. It is applied at 6 to 12 g ai/ha in autumn-sown cereals. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Rapid necrosis or desiccation of stems and leaves in the presence of light
Absorption/translocation: Contact herbicide with limited translocation
Mechanism of resistance in weeds: No resistance reported

BEHAVIOR IN SOIL

Sorption: 1480-2700 mL/g
Transformation:
Photodegradation: NA
Persistence:
Field Experiments: DT_{50} 1-7 d
Lab Experiments: NA
Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyraflufen-ethyl unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >5000mg/kg; slight eye irritation non-irritant to skin
Wildlife:
Carp LC_{50} (48-h), > 10 mg/kg; rainbow trout LC_{50} (48-h), > 10 mg/kg
Use classification: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry Source(s): Nichino America
Reference(s):

1. Miura, Y.M. Ohnishi, T. Mabuchi, and I. Yanai. 1993. ET-751; A new herbicide for use in cereals. Proc. 1993 Br. Crop Prot. Conf. – Weeds. Vol. 1: 35-40.

pyrazolynate

CAS #: 58011-68-0

27$^{(F_2)}$

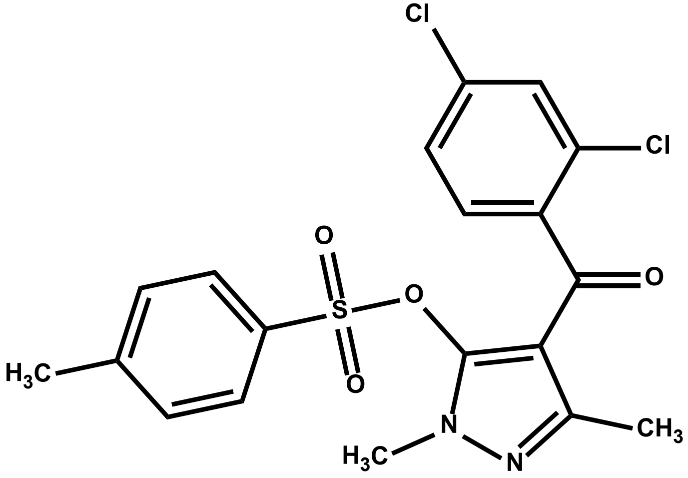
(2,4-dichlorophenyl)[1,3-dimethyl-5-[[(4-methyphenyl) sulfonyl]oxy]-1*H*-pyrazol-4-yl]methanone

NOMENCLATURE

Common name: pyrazolynate
Other name(s): pyrazolate; A-544; H-468T; SW-751; 4-(2,4-dichlorbenzoyl)-1,3-dimethylpyrazol-5-yl toluene-4-sulfonate
Trade name(s): SANBIRD
Chemical family: benzoylpyrazole; pyrazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *pyrazolynate*



Molecular formula: $C_{19}H_{16}Cl_2N_2O_4S$
Molecular weight: 439.31 g/mole
Description: Colorless, rod-shaped crystals
Density: NA
Melting point: 117-118.5 C
Boiling point: NA
Vapor pressure: <1.3 x 10^{-6} Pa (20 C)
Stability: Aqueous solutions hydrolyze readily
Solubility:
water 0.056 mg/L (25 C)
ethanol 14 g/L ethyl acetate 118 g/L
1,4-dioxane 256 g/L hexane 0.6 g/L
pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

Pyrazolynate is used for control of grasses, sedges, *Potamogeton distinctus*, *Sagittaria trifolium*, and *Alisma camaliculatum* in paddy rice; not marketed in U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme 4-hydroxyphenyl-pyruvate dioxygenase (4-HPPD) affecting carotenoid biosynthesis (more details on page 15)
Symptomology: Bleaching of affected plant tissue
Absorption/translocation: Absorbed by roots and translocated primarily by xylem
Metabolism in plants: NA
Mechanism of resistance in weeds: No resistance reported

BEHAVIOR IN SOIL

Persistence:
Field Experiments: DT_{50} in soil 10-20 d; microbially degraded by oxidative loss of sulfur to give 4-methylcatechol

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyrazolynate unless otherwise indicated.
Acute toxicity:
Oral LD_{50} male rat, 9550 mg/kg, female rat, 10233 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; Irritation to skin, none
Mutagenicity: Non-mutagenic
Wildlife:
LC_{50} for carp 92 mg/L

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Sankyo
Reference(s):

1. Roberts, T.R. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.

pyrazon

CAS #: 1698-60-8 **$5^{(C_1)}$**

5-amino-4-chloro-2-phenyl-3(2*H*)-pyridazinone

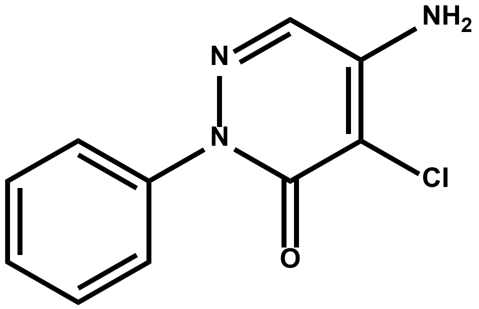
NOMENCLATURE

Common name: pyrazon (ANSI, BSI, ISO, WSSA)
Other name(s): chloridazon; BAS 119 H; 5-amino-4-chloro-2-phenylpyridazin-3(2*H*)-one (IUPAC)
Trade name(s): PYRAMIN®
Chemical family: pyridazinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

pyrazon



Molecular formula: $C_{10}H_8ClN_3O$
Molecular weight: 221.65 g/mole
Description: Yellow-brown crystalline solid, pyridine-like odor when pure
Density: 1.54 g/mL
Melting point: 207 C
Boiling point: NA
Vapor pressure: 1.01×10^{-5} Pa (56.5 C)
Stability: Relatively stable to UV light; Decomposes at 207 C
Solubility: water 400 mg/L (20 C)
pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

Pyrazon can be applied PRE at 3.49-8.53 kg ai/ha or early POST at 3.53-4.12 kg ai/ha in sugarbeets, and PRE at 3.53-4.12 kg ai/ha or early POST at 4.12 kg ai/ha in red table beets. It controls several annual broadleaf weeds including lambsquarters, pigweed spp., shepherd's-purse, annual smartweed spp., and purslane.

USE PRECAUTIONS

Fire hazard: Non-flammable
Corrosiveness: Non-corrosive
Storage stability: No limitations
Cleaning glassware/spray equipment: Wash with water and detergent.
Incompatibilities: Generally compatible with other sugarbeet herbicides. When tank-mixing with liquid formulations, pyrazon should be fully suspended before adding the liquid herbicide.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II). (more details on page 13)
Symptomology: NA
Absorption/translocation: Moderately absorbed by foliage with little to no translocation from treated leaves. Foliar absorption is increased by a surfactant or oil adjuvant. Pyrazon is readily absorbed by roots and translocated to all plant parts, probably via the xylem (5, 6).
Metabolism in plants: Conjugation to form *N*-glucosyl pyrazon may be the basis for sugarbeet and red beet tolerance (7, 8).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Cross resistance of common lambsquarters, common groundsel, and smooth pigweed biotypes to pyrazon and several PS II herbicides suggests that resistance was due to decreased sensitivity to those herbicides at the level of photosynthetic electronic transport.

BEHAVIOR IN SOIL

Sorption: Adsorbs tightly to OM
K_{oc}: Average is 120 mL/g (10)
Transformation:
Photodegradation: Negligible losses
Other degradation: Microbial breakdown is moderately rapid depending on soil temperature and moisture. The primary degradation product is non-phytotoxic dephenylated pyrazon (1, 3).
Persistence: Short to moderate persistence with a typical field half-life of 21 d (10). Pyrazon provides 4-8 wk of weed control, depending on soil moisture and temperature.
Mobility: Increased leaching potential on sands and sandy loam soils
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyrazon unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, 2200 mg/kg; mouse, 3000 mg/kg; rabbit, 1250 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation rabbit, none
Subchronic toxicity:
90-d dietary, mouse: NOEL 300 mg/kg
105-d dietary, rat: NOEL NA; no effects at 5000 mg/kg
Chronic toxicity:
24-mo dietary, mouse: NOEL 1000 mg/kg
25-mo dietary, rat: NOEL 300 mg/kg
12-mo dietary, dog: NOEL 600 mg/kg

Teratogenicity:

Rabbit: NOEL 55 mg/kg/d

Reproduction:

Rat: NOEL 100 mg/kg in a 2-generation study

Mutagenicity: Not mutagenic in unspecified tests

Wildlife:

Bluegill sunfish 96-h LC_{50}, ~40 mg/L; Fathead minnow LC_{50}, ~40 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: The condensation of mucochloric acid with phenyl hydrazine produces 1-phenyl-4,5-dichloropyridazone-6. Subsequent reaction with ammonia produces pyrazon.

Purification of technical: Recrystallize from methanol-water.

Analytical methods: Separate determination of pyrazon and metabolites using TLC and GLC (details from the manufacturer)

Historical: The first experimental results in Europe were published by Fischer. U.S. development began in 1963. U.S. patent 3,210,353 was assigned to BASF.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF

Reference(s):

1. Drescher and Otto. 1969. Z. Pflanzenbrank. Pflanzensch. 76:27 (in German).
2. Eshel, Y. 1969. Weed Res. 9:167.
3. Frank and Switzer. 1969. Weed Sci. 17:323.
4. Frank and Switzer. 1969. Weed Sci. 17:344.
5. Frank and Switzer. 1969. Weed Sci. 17:365.
6. Koren and Ashton. 1973. Weed Sci. 21:241.
7. Ries, S. K. et al. 1968. Weed Sci. 16:40.
8. Stephenson and Ries. 1969. Weed Sci. 17:327.
9. Tischer and Strotmann. 1977. Biochim. Biophys. Acta 314:113.
10. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

pyrazosulfuron-ethyl

CAS #: 93697-74-6 $2^{(B)}$

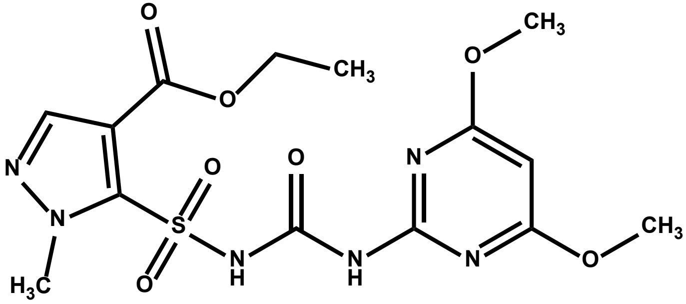
ethyl 5-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]
amino]sulfonyl]-1-methyl-1*H*-pyrazole-4-carboxylate

NOMENCLATURE

Common name: pyrazosulfuron-ethyl (ISO)
Other name(s): NC-311; ethyl 5-[(4,6-dimethoxypyrimidin-2-ylcarbamoyl)sulfamoyl]-1-methylpyrazole-4-carboxylate (IUPAC)
Trade name(s): ACT; AGEEN; BILLY; SIRIUS®; SPARKSTER
Chemical family: pyrazole; pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
pyrazosulfuron-ethyl



Molecular formula: $C_{14}H_{18}N_6O_7S$
Molecular weight: 414.39 g/mole
Description: Colorless crystals
Density: 1.44 g/mL (20 C)
Melting point: 181-182 C
Vapor pressure: 14.7 Pa (20 C) and stable
Stability: Stable (50 C) for 6 mo
Solubility:

water 14.5 mg/L (20 C)
methanol 0.2 hexane 0.2
benzene 15.6 acetone 31.7
hexane 0.2 g/L (20 C)

pK$_a$: NA
K$_{ow}$: log K_{ow} = 1.3

HERBICIDAL USE

Pyrazosulfuron-ethyl is used for preemergence and postemergence control of annual broadleaf weeds as well as annual and perennial sedges in rice.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Cessation of growth and chlorosis of treated plants.
Absorption/translocation: Absorbed by roots and shoots; primarily phloem mobile.
Metabolism in plants: The primary metabolite is the *O*-demethylated metabolite of pyrazsulfuron-ethyl.
Mechanism of resistance in weeds: Altered target site

BEHAVIOR IN SOIL

Sorption: NA
Transformation:

Photodegradation: NA
Other degradation: Unstable in acidic or alkaline media because of cleavage of sulfonylurea bridge. Soil DT_{50} <15 d. The main degradates found are hydrolysis product of ethyl ester to pyrazosulfuron-ethyl as well as *O*-demethylated products.

Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyrazosulfuron-ethyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rats, 2079-2349 mg/kg for male rats and 2205 mg/kg for female rats; Inhalation LC_{50} (rats), 3.9 mg/L; non-irritating to skin or eyes

Subchronic toxicity:

90-d dietary, rat: NOEL 400 mg/kg

Teratogenicity:

Rat: Non-teratogenic

Mutagenicity: Ames test, negative
Wildlife:

Acute oral LD_{50} bobwhite quail, >2250 mg/kg; rainbow trout and bluegill sunfish LC_{50} (96-h), >180 mg/L, carp (48-h), >30 mg/L; bees LD_{50} (contact), >100 µg/bee

Use classification: WHO class V; EPA (formulated) III

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Nissan Chemical Industry
Reference(s):

1. Roberts, T. R. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.

pyrazoxyfen

(2-[[4-(2,4-dichlorobenzoyl)-1,3-dimethyl-1*H*-pyrazol-5-yl] oxy]-1-phenylethanon

CAS #: 71561-11-0

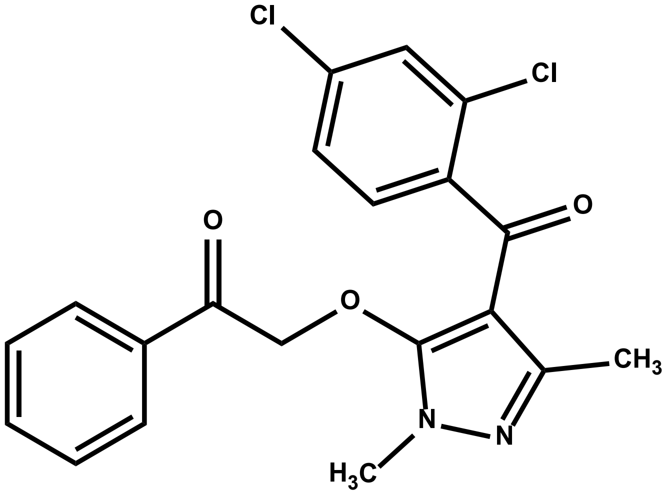
$27^{(F_2)}$

NOMENCLATURE

Common name: pyrazoxyfen (ISO approved)
Other name(s): SL-49; 2-[4-(2,4-dichlorbenzoyl)-1,3-dimethylpyrazol-5-yloxy]acetophenone (IUPAC)
Trade name(s): PAICER
Chemical family: benzoylpyrazole; pyrazole

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *pyrazoxyfen*



Molecular formula: $C_{20}H_{16}Cl_2N_2O_3$
Molecular weight: 403.26 g/mole
Description: Colorless crystals
Density: 1.37 g/mL (20 C)
Melting point: 111-112 C
Vapor pressure: 4.8 x 10^{-5} Pa (25 C)
Stability: Stable to acid, alkali, light and heat
Solubility:

water 0.9 g/L (20 C)
acetone 223 g/L
ethanol 14 g/L
hexane 900 g/L
toluene 200 g/L
benzene 325 g/L
chloroform 1068 g/L
xylene 116 g/L

pK_a: None (non-ionizable)
K_{ow}: NA

HERBICIDAL USE

Pyrazoxyfen is used for pre- or post-emergence, after transplanting, in paddy rice to control annual and perennial weeds. It can be used in direct- seeded rice; cannot be used successfully in upland crops. Use rates are 3 kg ai/ha. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme 4-hydroxyphenyl-pyruvate dioxygenase (4-HPPD) affecting carotenoid biosynthesis (more details on page 15)
Symptomology: Bleaching and chlorosis of affected plant tissue.
Absorption/translocation: Absorbed by young stems and roots of weeds and translocated primarily by the xylem.
Metabolism in plants: NA
Mechanism of resistance in weeds: No resistance has been reported.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:

Other degradation: DT_{50} 4-15 d. Degradation is more rapid in mineral soils (DT_{50} 3-5 d) than in volcanic ash (DT_{50} 5-34 d) and pyrazoxyfen degradation took place more rapidly under flooded conditions.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyrazoxyfen unless otherwise indicated.
Acute toxicity:

Oral LD_{50} male rat, 1690 mg/kg; female rat, 1644 mg/kg; Dermal LD_{50} rat, >5000 mg/kg LC_{50} (48 h) carp, 2.5mg/L; rainbow trout 0.79mg/L; killfish 2.7 mg/L; Daphnia LC_{50} (3h), 127 mg/L

Use classification: WHO class III, EPA (formulation) III.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Syngenta Crop Protection
Reference(s):

1. Roberts, T.R. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.

pyribenzoxim

CAS #: 168088-61-7 $2^{(B)}$

diphenylmethanone *O*-[2,6-bis(4,6-dimethoxy-2-pyrimidinyl) oxy)benzoyl]oxime

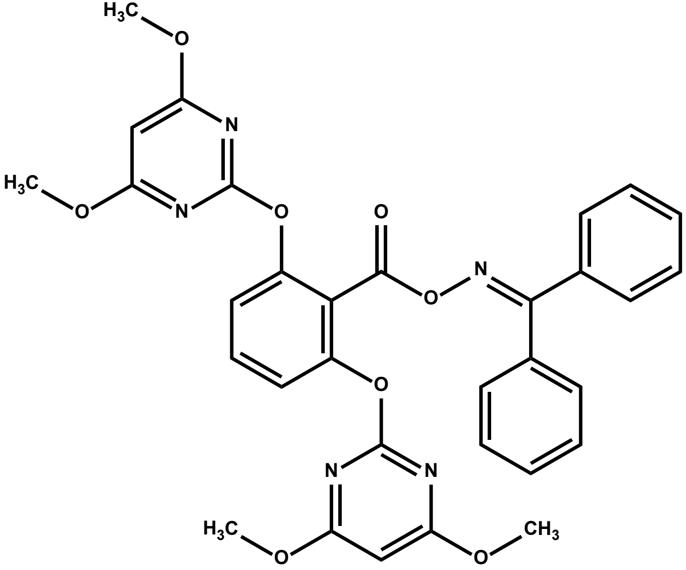
NOMENCLATURE

Common name: pyribenzoxim (ISO proposed)
Other name(s): LGC-40863; benzophenone *O*-[2,6-bis(4,6-dimethoxypyrimidin-2-yloxy)benzoyl]oxime
Trade name(s): PYANCHORO
Chemical family: Unclassified

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure

pyribenzoxim



Molecular formula: $C_{32}H_{27}N_5O_8$
Molecular weight: 609.60 g/mole
Description: Odorless white powder
Density: NA
Melting point: 128 - 130 C
Boiling point: NA
Vapor pressure: 9.8 x 10^{-4} Pa
Stability: Stable to UV light; little or no decomposition after 30 d (100 C)
Solubility:
water 3.5 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 1.63 ethanol 0.55
n-hexane 0.04 ether 0.97
acetonitrile 10.82 solvesso #100 1.85
toluene 11.08xylene 3.81
cyclohexane 23.67 methanol 0.472
benzene 42.65
methylene chloride 4.52
dimethylformamide 10.48
pK_a: NA (non-ionizable)
K_{ow}: 3.04

HERBICIDAL USE

Pyribenzoxim is a POST herbicide selective to rice, turfgrass, and winter cereals. The use rate is at 30 to 70 g ai/ha depending on the crop. In rice, the herbicide controls certain annual grasses, many broadleaf weeds, and sedges including barnyardgrass, alexandergrass, winklegrass, large crabgrass, Indian jointvetch, hemp sesbania, smartweed, morningglory, redstem, common dayflower, marsh dayflower, arrowhead, flat sedge, umbrella plant, and bulrush (1-3). The herbicide also controls blackgrass in winter cereals and annual bluegrass in turfgrass.

USE PRECAUTIONS

Fire hazard: Technical ingredient is dry and non-flammable. The product PYANCHOR is flammable; flash point is 42.5 C.
Corrosiveness: PYANCHOR is non-corrosive to metals.
Storage stability: Shelf life is > 2 yr for PYANCHOR.
Cleaning glassware/spray equipment: Wash with water
Incompatibilities: Contact-type herbicides are usually antagonistic for grass control.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12).
Symptomology: Elongation of new leaves is inhibited as early as 24 h after treatment. Treated plants are stunted and become chlorotic 3 to 5 days after treatment, followed by complete plant desiccation 15 to 20 days after treatment.
Absorption/translocation: About 50 to 60% of the treated herbicide is absorbed by foliage, and 5 to 7% of the total treated radiolabel is translocated toward upper leaves and roots.
Metabolism in plants: Results show that rice tolerance is due to metabolism.
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: Pyribenzoxim binds strongly to soil
K_{oc}: 5.9 x 10^5 mL/g for a loamy sand with 1.7% OM and pH 4.3; 5.15 x 10^5 mL/g for a silty clay with 1.6% OM and pH 4.8; 8.57 x 10^4 for a clay with 2.5% OM and pH 5.9; 2.47 x 10^6 for a silt loam with 0.7% OM and pH 7.7

BEHAVIOR IN SOIL

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Transformation:
Photodegradation: Negligible
Other degradation: Microbial degradation

Persistence: Field half life is about 7 d
Mobility: Remains in top 5 cm of soil
Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyribenzoxin unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; Primary eye irritation rabbit, non irritant; Skin sensitization guinea pig, negative

Subchronic toxicity:

90-d Oral, rat: NOEL >2000 mg/kg
21-d Dermal, rat: NOEL >1000 mg/kg

Chronic toxicity: NA

Teratogenicity:

Rat: Non-teratogenic >2000 mg/kg

Reproduction: NA

Mutagenicity:

Gene mutation: Ames test, negative
Structural chromosome aberration: Mouse micronucleus, negative

Wildlife:

Honey bee 24-h LD_{50}, >100 mg/bee; Daphnia, 48-h LC_{50}, >100 mg/L; carp LC_{50}, >10 mg/L; Madeka, 96-h LC_{50}, >100 mg/L; algae 96-h LC_{50}, >100 mg/L

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: Available on request
Analytical methods: HPLC methods are available on request.
Historical: First synthesized in 1992 by LG Chemical Ltd.; commercialized in 1997 (Korea)

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): LG Chemical

Reference(s):

1. Cho, J. H. et al. 1997. Proc. Brighton Crop Prot. Conf. Weeds, pp. 39-44.
2. Bae, Y. T. et al. 1997. Kor. J. Weed Sci. Soc. Am. 37:66.
3. Lim, J. S. et al. 1997. Abstr. Weed Sci. Soc. Am. 37:66.

pyridate

CAS #: 55512-33-9

$6^{(C_3)}$

O-(6-chloro-3-phenyl-4-pyridazinyl) *S*-octyl carbonothioate

NOMENCLATURE

Common name: pyridate (BSI, ISO, WSSA)

Other name(s): CL 11344; *O*-6-chloro-3-phenylpyridazin-4-yl *S*-octyl thiocarbonate (IUPAC)

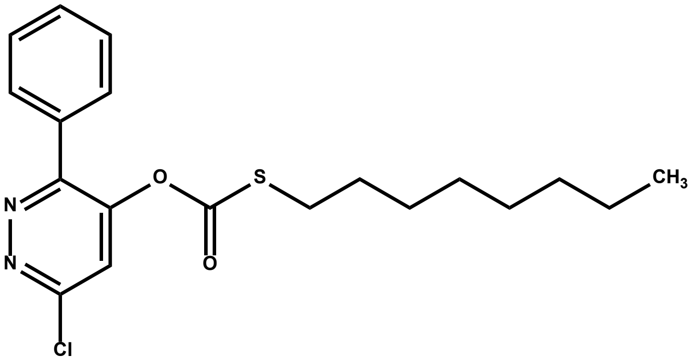
Trade name(s): LENTAGRAN; PYRON; TOUGH

Chemical family: phenylpyridazine; pyridazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

pyridate



Molecular formula: $C_{19}H_{23}ClN_2O_2S$

Molecular weight: 378.92 g/mole

Description: White crystalline solid when pure; technical is a brown, oily liquid

Density: 1.56 g/mL (20 C) (technical)

Melting point: 27 C

Boiling point: >220 C (14 Pa)

Vapor pressure: 1.34 x 10^{-5} Pa (20 C)

Stability: Not degraded by UV light

Solubility:

water 1.5 mg/L (20 C)

organic solvents g/100 mL (20 C):

acetone >10	methanol >12
benzene >10	toluene >10

pK$_a$: None (non-ionizable)

K$_{ow}$: >1000

HERBICIDAL USE

Pyridate can be applied at-cracking at 1.05 kg ai/ha or POST at 1.05-1.6 kg ai/ha in peanuts, and POST at 0.53-1.05 kg ai/ha in corn. It also is sold in Europe on cereals, rice, turf, grassland, poppies, onions, leeks, alfalfa, red clover, chickpeas, cole crops, oilseed rape, asparagus, orchards, vineyards, and on pines, spruces, and firs.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are non-flammable.

Corrosiveness: Non-corrosive

Storage stability: Stable for >25 mo according to WHO regulations; store under dry and freeze-free conditions

Cleaning glassware/spray equipment: Warm water and/or organic solvents

Emergency exposure: If ingested, induce vomiting and seek medical advice. No antidote known

Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Pyridate is hydrolyzed to 3-phenyl-4-hydroxy-6-chloropyridazine which then inhibits photosystem II in the electron transport chain of photosynthesis (more details on page 13)

Symptomology: Withering begins at the leaf edges and is complete within 5-10 d in susceptible species

Absorption/translocation: Rapidly absorbed by foliage (>90% in 6 h), but poorly translocated. Pyridate efficacy is unaffected by rain occurring 1 h after application.

Metabolism in plants: Rapidly hydrolyzed (half-life ranging from a few minutes to days) to 3-phenyl-4-hydroxy-6-chloropyridazine, followed by conjugation to form non-phytotoxic *O*- and *N*-glycosides.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to soil

K$_d$: 0.3-26 mL/g for the primary metabolite, 3-phenyl-4-hydroxy-6-chloropyridazine

Transformation:

Photodegradation: Negligible losses of pyridate, but the primary metabolite, CL 9673 (3-phenyl-4-hydroxy-6-chloropyridazine), has a half-life of 6-7 d

Other degradation: Rapidly hydrolyzed to CL 9673 with a half-life of 0.5-1.5 d. CL 9673 is then biologically degraded.

Persistence: Non-persistent

Field experiments: Half-life ranges from 7-21 d

Lab experiments: Half-life ranges from 33-43 d

Mobility: Immobile in soil

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyridate unless otherwise indicated.

Acute toxicity:

Oral LD$_{50}$ rat, 4690 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; 4-h inhalation LC$_{50}$, >4.37 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, yes; Eye irritation rabbit, none

TOUGH 45 WP: Oral LD$_{50}$ rat, 2330 mg/kg; Dermal LD$_{50}$ rabbit, >2000 mg/kg; 4-h inhalation LC$_{50}$, >2.14 mg/L (highest attainable conc.); Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, yes (reversible in 7 d)

TOUGH 3.75 EC: Oral LD_{50} rat, 2813 mg/kg; Dermal LD_{50} rabbit, >4000 mg/kg; 4-h inhalation LC_{50}, >6.56 mg/L; Skin irritation rabbit, yes; Skin sensitization guinea pig, yes; Eye irritation rabbit, yes

Subchronic toxicity:

90-d dietary, rat: NOEL 62.5 mg/kg/d

90-d dietary, dog: NOEL 20 mg/kg/d

Chronic toxicity:

24-mo dietary, rat: NOEL 10.8 mg/kg/d; not carcinogenic

12-mo dietary, dog: NOEL 20 mg/kg/d; not carcinogenic

Teratogenicity:

Rat: NOEL developmental >495 mg/kg/d; not teratogenic

Rabbit: NOEL developmental >600 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL developmental 10.8 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Mouse micronucleus, negative; CHO/cytogenetics, negative

DNA damage/repair: Sprague Dawley rat/*In vivo* and *in vitro* UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >1269 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck 8-d dietary LC_{50}, >5000 mg/kg; Earthworm LC_{50} in soil, 799 mg/kg; Honey bee oral LD_{50}, 100 µg/bee, topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 1.08 mg/L; Bluegill sunfish 96-h LC_{50}, >2.1 mg/L; Rainbow trout 96-h LC_{50}, >2.1 mg/L

TOUGH 45 WP: Japanese quail oral LD_{50}, >2000 mg/kg; Earthworm LC_{50} in soil, >1000 mg/kg; Honey bee oral LD_{50}, >100 µg/bee, topical LD_{50}, >160 µg/bee; Daphnia 48-h LC_{50}, 3.3-7.1 mg/L; Carp 96-h LC_{50}, 187 mg/L; Rainbow trout 96-h LC_{50}, 114 mg/L

TOUGH 3.75 EC: Japanese quail oral LD_{50}, >2000 mg/kg; Earthworm LC_{50} in soil, >1000 mg/kg; Honey bee oral LD_{50}, >111 µg/bee, topical LD_{50}, >111 µg/bee; Daphnia 48-h LC_{50}, 0.9 mg/L; Carp 96-h LC_{50}, 45.4 mg/L; Rainbow trout 96-h LC_{50}, 13.9 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: 3-phenyl-pyridazone-6 is chlorinated and then saponified to produce 3-phenyl-4-hydroxy-6-chloropyridazine which is further reacted to produce pyridate.

Purification of technical: Distillation

Analytical methods: Available on request

Historical: Pyridate was discovered in 1974 at Chemie Linz AG, Austria. Formulated products are registered worldwide. EUP trials were conducted in the U.S. in 1987 and 1988 and in Canada in 1988.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Zohner, A. 1987. Proc. Brit. Crop Prot. Conf.-Weeds p. 1083.

pyrithiobac-sodium

CAS #: 123343-16-8 **2$^{(B)}$**

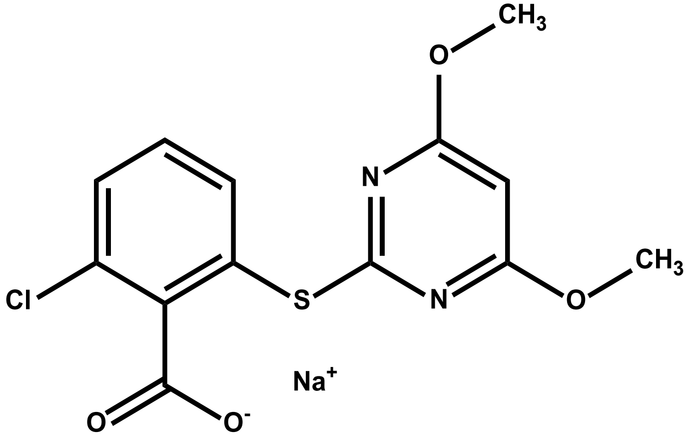
sodium 2-chloro-6-[(4,6-dimethoxy-2-pyrimidinyl)thio] benzoic acid

NOMENCLATURE

Common name: pyrithiobac (ANSI, ISO, WSSA)
Other name(s): DPX-PE350; KIH-2031 (Na salt); KIH-8921 (free acid); sodium 2-chloro-6-(4,6-dimethoxypyrimidin-2-ylthio)benzoate (IUPAC)
Trade name(s): PYRIMAX; STAPLE®; STAPLE® PLUS
Chemical Family: pyrimidinylthiobenzoic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
pyrithiobac-sodium



Molecular formula: $C_{13}H_{10}ClN_2NaO_4S$
Molecular weight: 348.74 g/mole
Description: Yellowish-white solid; slight garlic-like odor
Density: 0.47 g/mL (20 C)
Melting point: 246-250 C
Boiling point: NA
Vapor pressure: 4.8 x 10^{-8} Pa (25 C)
Stability: Stable at normal temperatures and storage conditions.
Solubility:
water 760 g/L (pH 4.5, 10 C)
pK$_a$: 2.34 (weak acid)
K$_{ow}$: log K_{ow} = (pH 5); $^{-}$0.84 (pH 7)

HERBICIDAL USE

Pyrithiobac-sodium is used POST in cotton at 35-105 g ai/ha for the control of a wide range of broadleaf weeds and some grasses. Pyrithiobac-sodium can also be used PRE at 35 g ai/ha for control of a number of small seeded broadleaf weeds. It provides excellent control of morningglories, common cocklebur, velvetleaf, prickly sida, hemp sesbania, nightshades, and johnsongrass.

USE PRECAUTIONS

Fire hazard: Not a fire or explosive hazard
Corrosiveness: Non-corrosive
Storage stability: Technical and formulated products are stable. Store product in original container and in a well-ventilated place. Do not store or consume food, drink or tobacco in areas where they may become contaminated with this material.
Cleaning glassware/spray equipment: Wash lab equipment with water and detergent, then rinse with acetone. Wash spray equipment with water and ammonia at 1% v/v and triple rinse with water. Do not contaminate water, other pesticides, fertilizer, food, or feed in storage.
Emergency exposure: Avoid contact with eyes, skin, or clothing. Wash thoroughly after handling. Avoid breathing dust. Wash hands before eating, drinking, chewing gum, using tobacco, or using the toilet. Flush eyes with plenty of water for at least 15 min, if eyes are exposed to the product. Wash skin with soap and water. If inhaled, expose individual to fresh air. If not breathing giving artificial respiration. If breathing is difficult, give oxygen. If ingested, immediately give 2 glasses of water, induce vomiting. Never give anything by mouth to an unconscious person.
Incompatibilities: Do not tank mix STAPLE® with Dual herbicide as a postemergence treatment as crop injury may result. Do not tank mix STAPLE® with malathion-containing insecticides as crop injury may result. To avoid crop injury, apply malathion-containing insecticide at least 24 h before or after application of STAPLE®.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Rapid growth inhibition of sensitive species occurs with POST applications. Injury symptoms vary by species and generally include chlorosis and necrosis of the meristematic region followed by general foliar chlorosis, necrosis and plant death.
Absorption/translocation: The herbicide can be absorbed following foliar and soil application and translocates primarily in the phloem of treated broadleaf plants.
Metabolism in plants: Cotton exhibits good tolerance to pyrithiobac following PRE or POST applications. Details on the metabolic pathways involved in the metabolism of this herbicide are not available.
Non-herbicidal biological properties: None identified.

BEHAVIOR IN SOIL

Sorption: Weakly absorbed
Transformation:
Photodegradation: Photochemical breakdown plays a major role in the degradation of pyrithiobac.
Other degradation: Microbial degradation plays a major role in the soil degradation of pyrithiobac.
Persistence: Pyrithiobac-sodium degrades slowly in soil, primarily by microbially mediated degradation, with

an estimated half-life of approximately 60 d in laboratory studies.

Mobility: Generally greater at higher soil pH and lower organic matter control.

Volatilization: Very low volatility

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyrithiobac-sodium unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat (male), 1000-3000 mg/kg, rat (female), 3000-5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; inhalation 4-h LC_{50} rat, > 5.6 mg/L; primary eye irritation rabbit, irritating; dermal irritation rabbit, negative, skin sensitization, guinea pig, negative

Subchronic toxicity:

90-d dietary, rat: 10 mg/kg (male), 500 mg/kg (female)

90-d-dietary, mouse: 500 mg/kg (male and female)

90-day dietary, dog: 5000 mg/kg

Chronic toxicity:

Rat: NOEL (maternal) 200 mg/kg/d, (fetal) 600 mg/kg/d; NOEL (2-generation for rat reproduction) 1500 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: Study with CHL cells was positive with/without S9 mix

Other tests: *In vivo* micronucleus test in mice was negative

Wildlife:

Aquatic: 96-h LC_{50} bluegill sunfish, >930 mg/L, rainbow trout, >1000 mg/L, sheepshead minnow, >145 mg/L, mysid shrimp, >140 g/L; 48-h EC_{50} Daphnia magna, >1100 mg/L; 96-h EC_{50} oyster shell deposition, >130 mg/L

Avian/Honeybee: Oral LD_{50}, 1599 mg/kg; 5-d LC_{50} bobwhite quail, >5620 mg/kg; Mallard duck, >5620 mg/kg; Contact LD_{50} honeybee, >25 μg/bee

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Pyrithiobac was discovered in Japan by KUMIAI (US Patent No. 4,932,999). It was licensed for development by Du Pont in 1990. The product was registered for use in the US in 1996.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; DuPont Crop Protection

pyroxasulfone

CAS #: 447399-55-5

15$^{(K_3)}$

3-[5-(difluoromethoxy)-1-methyl-3-(trifluoromethyl)pyrazol-4-ylmethylsulfonyl]-4,5-dihydro-5,5-dimethyl-1,2-oxazole

NOMENCLATURE

Common name: pyroxasulfone (ISO)

Other name(s): KIH-485, 5-(difluoromethoxy)-1-methyl-3-(trifluoromethyl)pyrazol-4-ylmethyl 4,5-dihydro-5,5-dimethyl-1,2-oxazol-3-yl sulfon (IUPAC)

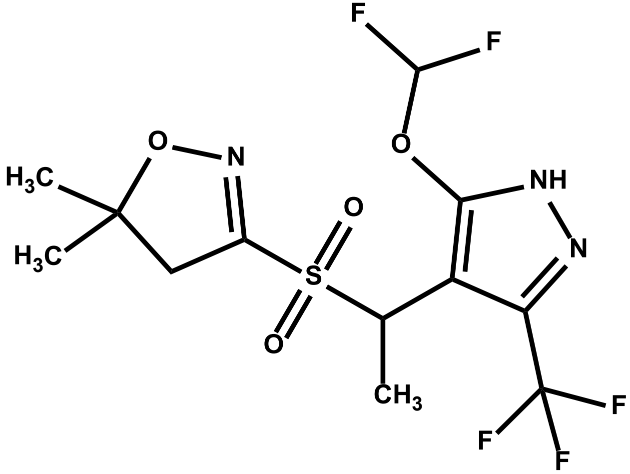
Trade name(s): SAKURA, ZIDUA® FIERCE™; ANTHEM™

Chemical family: isoxazoline

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

pyroxasulfone



Molecular formula: $C_{12}H_{14}F_5N_3O_4S$

Molecular weight: 391.316 g/mol

Description: White crystal solid

Density: 1.60 g/cm^3

Melting point: 130.7 ℃

Boiling point: Unknown

Vapor pressure: 2.4×10^{-6} Pa (25 ℃)

Stability: Stable at room temperature

Solubility:

water 3.49 mg/L (20 C)

pK$_a$: None (non-ionizable)

K$_{ow}$: Log P_{ow}=2.39 (25 ℃)

HERBICIDAL USE

Pyroxasulfone (HRAC Group K3, WSSA Group 15) is a selective herbicide for control of grasses and small-seeded broadleaves such as Italian ryegrass, barnyardgrass, foxtails, crabgrasses, Palmer amaranth, and common waterhemp in corn, wheat and soybeans. Pyroxasulfone can be used from fall through early preplant to early postemergence for control of troublesome weeds including resistant weeds to glyphosate, ALS-inhibitors, ACCase-inhibitors and triazines with residual control.

USE PRECAUTIONS

Fire hazard: Technical and formulated pyroxasulfone are non-flammable

Corrosiveness: Formulated products are non-corrosive

Storage stability: Good stability. Store in cool, dry place and avoid excess heat. Store in original containers only. Keep out of reach of children and animals. Do not contaminate water, food or feed by storage or disposal.

Cleaning glassware/spray equipment: Clean glassware and equipment with a solution of soap and water. Avoid contamination of water by cleaning of equipment or disposal of wastes. Large spills should be covered to prevent dispersal.

Emergency exposure: If ingested, drink 1-2 glasses of water. Do not induce vomiting or give anything by mouth to an unconscious individual. Contact a medical doctor. If inhaled, remove to fresh air. If breathing discomfort occurs, contact a medical doctor. For skin and eye exposure wash with plenty of soap and water or flush with water for at least 15 minutes. If irritation occurs or persist get medical attentions.

Incompatibilities: Pyroxasulfone has been found to be physically compatible with most commercially available herbicides.

BEHAVIOR IN PLANTS

Mechanism of action: Pyroxasulfone treatment drastically reduces the biosynthesis of very-long-chain fatty acids (VLCFAs) and causes a buildup of fatty acid precursors. Pyroxasulfone specifically inhibits many elongation steps catalyzed by VLCFA elongases. (more details on page 14)

Symptomology: Most susceptible grass and broadleaf weeds fail to emerge because the growth of apical meristem and coleoptile are interrupted after germination. Susceptible monocots that do emerge appear twisted and malformed with leaves tightly rolled in the whorl and unable to unroll normally. Broadleaf seedlings may have slightly cupped or crinkled leaves and shortened leaf midribs producing a drawstring effect on the leaf tip..

Absorption/translocation: Most susceptible grass and broadleaf weeds fail to emerge because the growth of apical meristem and coleoptile are interrupted after germination. Susceptible monocots that do emerge appear twisted and malformed with leaves tightly rolled in the whorl and unable to unroll normally. Broadleaf seedlings may have slightly cupped or crinkled leaves and shortened leaf midribs producing a drawstring effect on the leaf tip.

Metabolism in plants: Thiazopyr??? (comment: this paragraph needs to be rewritten) is extensively and rapidly degraded to a large number of polar metabolites, each comprising <10% of the total applied thiazopyr??? residues. Major degradation reactions include sulfur oxidation, thiazoline ring opening and methyl ester hydrolysis, and transformation of the isobutyl side chain. The 2-difluoromethyl-4-(2-methylpropyl)-6-trifluoromethyl-3-(pyridinecarboxylate moiety is found in most of the metabolites as well as in the parent thiazopyr.

Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to soil. K_{oc} ads 57-114, K_{oc} des 119-226

rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >1.2 mg/L; (comments: this should be in next section)

Photo degradation: Negligible losses
Other degradation: Hydrolytically stable at pH 5, 7 and 9. Microbial degradation is a major contributor to field dissipation.
Persistence: Pyroxasulfone is not persistent in soils. Terrestrial field dissipation Half-life: 16-26 days
Mobility: Pyroxasulfone has low leaching potential. It is less mobile in fine and medium textured soils and more mobile in coarse textured soils.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyroxasulfone unless otherwise indicated.

Acute toxicity
Acute Oral LD_{50} Rats: LD_{50} >2000 mg/kg
Acute Dermal LD_{50} Rats: LD_{50} >2000 mg/kg
Acute Inhalation LC_{50} (dust, 4h) Rats: LC_{50} >6.56 mg/L
Primary Eye Irritation Rabbits: Minimally irritating (not classified)
Primary Dermal Irritation Rabbits: non-irritating
Dermal Sensitization Mouse (LLNA): No sensitization

Subchronic and Chronic toxicity
Increase of AST, slightly weigh gain of liver and kidney, increase of cardiomyopathy, centrilobular hypertrophy of hepatocyte and hyperplastic of urinary bladder mucosa were observed in male and female rat study, and no effect was observed at 50 ppm (male: 2.22 mg/kg/day and female: 3.12 mg/kg/day).

Increased incidence of urinary bladder transitional cell papillomas was reported in male rat in carcinogenicity study.

Teratogenicity and Reproduction
Pyroxasulfone was not considered to be a reproductive toxicant in rats or teratogenic in rats and rabbits.

Mutagenicity
Pyroxasulfone was not considered to be a genotoxicant based on the negative results of all mutagenicity studies.

Wildlife:
Fish (Rainbow Trout) LC50 (96h) >2.2 mg/L; (Bluegill) LC50 (96h) >2.8 mg/L; (Sheepshead minnow) LC50 (96h) >3.3 mg/L; Daphnia magna EC50 (48h) >4.4 mg/L; Algae ErC50 (96h) 0.00079 mg/L; Duck weed EC50 (7days) 0.0055 mg/L; Earthworm LC50 (14days) >997 mg/kg; Honeybee Acute contact LD50 (48h) >100 µg/bee; Avian (Bobwhite quail) Acute oral LD50 >2250 mg/kg bw

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA.

Historical: Pyroxasulfone has been discovered and being developed by Kumiai Chemical Industry Co., Ltd and Introduced to the U.S by BASF, Valent and FMC.

I

MANUFACTURER(S) AND INFORMATION SOURCES:

Information Sources: K-I Chemical USA
Reference(s):

1. Tanetani Y. et al. 2009. Action mechanism of a novel herbicide, pyroxasulfone. Pesticide Biochem. Physio. 95:47–55.

pyroxsulam

CAS #: 422556-08-9 $2^{(B)}$

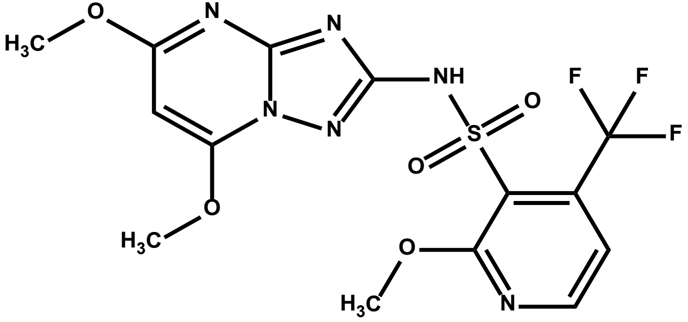
N-(5,7-dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)
-2-methoxy-4-(trifluromethyl)pyridine-3-sulfonamide

NOMENCLATURE

Common Name: pyroxsulam
Other names: DE-742, XDE-742, XR-742, X666742, CA N-(5,7-dimethoxy[1,2,4]triazolo[1,5-a] pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide.
Trade Names: POWERFLEX®, SIMPLICITY®, PARADIGM® (USA), FLORAMIX®, HURRICANE® (EU)
Chemical Family: triazolopyrimidine sulfonamide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical Structure:
Pyroxsulam



Molecular formula: $C_{14}H_{13}F_3N_6O_5S$
Molecular weight: 434.354 amu
Description: technical active ingredient is an off-white powder
Density: 1.618g/cm^3 at 20ºC
Melting point: Melts with decomposition at 208 C
Vapour pressure: Less than $1x10^{-7}$Pa at 20ºC
Solubility (g/L at 20ºC): Distilled water 0.0626, pH 4 Buffer 0.0164, pH 7 Buffer 3.20, pH 9 Buffer 13.7, Acetone 2.79, Ethyl Acetate 2.17, 1,2-Dichloroethane 3.94, Methanol 1.01, Octanol 0.0730, Xylene 0.0352 and Heptane <0.001
pKa: 4.67 weak acid
Kow (log Kow @ 20ºC) : pH 4 = 1.08, pH 7 = -1.01, pH 9 = -1.60

HERBICIDAL USE

Pyroxsulam is a triazolopyrimidine sulfonylanilid herbicide that provides broad spectrum postemergence annual grass and broadleaf weed control in cereals. Pyroxsulam provides control of key annual grasses including *Alopecurus* spp., *Apera spica-venti, Avena* spp., *Bromus* spp., *Lolium* spp., and others. Pyroxsulam also provides control of key broadleaves in cereals including *Amaranthus* spp., *Brassica* spp., *Galeopsis tetrahit, Geranium* spp., *Myosotis arvensis, Stellaria media, Veronica* spp., and *Viola tricolor.* Pyroxsulam provides herbicidal activity at low use rates. Postemergence use rates in cereals will range from 9 -18.75 grams ai/hectare depending upon target weed species and geography postemergence application, however, it can also provide short soil residual control of newly emerging annual weeds.

USE PRECAUTIONS

Fire hazard: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: As a member of the triazolopyrimidine sulfonylanilid class of chemistry, pyroxsulam inhibits the plant enzyme acetolactate synthase (ALS). (more details on page 12)
Symptomology: Symptoms include stunting and chlorosis, followed by necrosis and then death. Plant injury symptoms from an application of pyroxsulam are typical of ALS inhibitor herbicides and will generally result in the following visual symptomology on susceptible weeds: almost immediate growth inhibition, chlorosis of leaves and growing point with some possible vein reddening in the first few days, necrosis of the apical meristem in approximately 7 to 14 days after application, plant death generally within 2 to 4 weeks under normal growing conditions and up to 6-8 weeks under prolonged adverse growing conditions. Weeds treated with pyroxsulam will stop growing almost immediately, and the competitive effect of the weeds with the cereal crop should be minimal following application. Complete plant death can be slow compared to some other products. The rate of plant death is likely related to the total pool of branched chain amino acids available; small plants will succumb much more rapidly than larger plant species with greater reserves. Adverse environmental conditions that slow plant metabolism (cold, dry) will slow the speed of kill. Field trial results indicate optimum weed control occurs when grass weeds are in the 1 to 5 leaf, 1 tiller growth stage.
Absorption/translocation: Pyroxsulam is a systemic, phloem and xylem mobile herbicide that is absorbed via leaves, shoots, and roots. The leaves and roots are the primary uptake sites in plants. The compound is translocated in plants to meristematic tissue.
Metabolism in plants: Pyroxsulam is a triazolopyrimidine sulfonylanilid whose mode of action is the inhibition of the acetolactate synthase enzyme (ALS) in plants. Other families of chemistries exist with the same mode of action, *i.e.* the sulfonylureas, the triazolinones and the imidazolinones.
Resistance: Cases of resistance to ALS inhibiting herbicides have been reported, particularly in cereals but also in rice. Most cases have occurred where there was a repeated use of ALS-inhibitor herbicides. These highly efficient products induce a very strong selection pressure. There are two types of resistance following selection with sulfonylureas: either a target site resistance (the target ALS enzyme is less sensitive to inhibition by the herbicide) or an enhanced metabolic resistance (the plant metabolism of the herbicide is increased, resulting in a rapid detoxification of this herbicide). There is a considerable variation in the level

of resistance across and within ALS-inhibiting herbicides.

BEHAVIOR IN SOIL

Sorption: Laboratory experiments yielded an average **K_{oc}** of 30 mL/g (range 2-129 mL/g), indicating that pyroxsulam is weakly to moderately adsorbed. However, field dissipation studies showed limited movement in the soil profile. Pyroxsulam is more tightly bound to organic matter than to clay and solubility increases with pH. Consequently, degradation rates are generally faster with higher pH and lower organic matter.

Transformation:

Photodegradation: Minor

Other degradation: Aerobic microbial degradation is the primary route of breakdown of pyroxsulam in soil.

Persistence: Pyroxsulam undergoes rapid aerobic microbial soil degradation with an average laboratory soil half-life of three (3) days at 20˚C. Field dissipation studies, conducted in-season in western Canada, resulted in an average soil half-life of 13-days. Pyroxsulam rapidly degrades and residues in the soil generally do not persist long enough to injure crops the following season. No degradation metabolites of concern were produced in any studies. Like many compounds which are microbially degraded, it requires adequate moisture and temperature for breakdown to occur.

Mobility: Field dissipation studies showed limited movement in the soil profile. Pyroxsulam is more tightly bound to organic matter than to clay and solubility increases with pH. Consequently, degradation rates are generally faster with higher pH and lower organic matter.

Volatilization: The potential for transport of pyroxsulam via volatilization of residues is extremely low, due to its low vapour pressure and small Henry's Law constant ($<1.36 \times 10^{-8}$ Pa m^3/mol at 20°C and pH 7). As with any herbicide, susceptible non-target plants may be injured via physical spray drift. Spray applications should be made such that spray drift cannot injure desirable, susceptible plant species.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade pyroxsulam unless otherwise indicated.

Acute toxicity: Based on data generated for, or on behalf of Dow AgroSciences, the acute mammalian toxicity of pyroxsulam is considered low for the technical active ingredient. Acute Oral Rat LD_{50} >2000 mg/kg Acute Dermal Rat LD_{50} >2000 mg/kg Acute Inhalation Rat LC_{50} >5.1 mg/L Dermal irritation Rabbit Not a dermal irritant Eye Irritation Rabbit Not an eye irritant Skin sensitization Guinea Pig Sensitizer

Chronic toxicity: Dow AgroSciences studies have shown that pyroxsulam (technical) is not carcinogenic, teratogenic, mutagenic, neurotoxic or a reproductive hazard. 2-year chronic feeding Rat Not carcinogenic NOAEL (mg/kg/day): 1000 Teratogenicity Rat Not teratogenic NOAEL (mg/kg/day): Maternal = 1000 Developmental = 1000 Teratogenicity Rabbit Not teratogenic NOAEL (mg/kg/day):

Maternal = 300 (highest dose tested) Developmental = 300 (highest dose tested) Reproductive toxicity Rat No adverse reproductive effects NOAEL (mg/kg/day): Parental = 1000 Reproductive = 1000 Chronic neurotoxicity Rat No adverse neurological effects NOAEL (mg/kg/day) = 1000

Mutagenicity: Mutagenicity Assay (in vitro) Ames test Negative, Mutagenicity Assay (in vitro) CHO/HGPRT Negative, Mutagenicity Assay (in vitro) RLCAT Negative, Mutagenicity Assay (in vitro) Mouse micronucleus Negative

Wildlife: In laboratory testing, pyroxsulam has been shown to be practically non-toxic to birds, fish, honeybees, earthworms and aquatic invertebrates. Pyroxsulam is moderately toxic to green and blue-green algae and aquatic higher plants (*Lemna gibba*), depending on the species.

Avian oral Bobwhite Quail LD_{50} >2000 mg ai/kg bw; Avian oral Mallard Duck LD_{50} >2000 mg ai/kg bw

Avian dietary Bobwhite Quail LC_{50} >5000 mg ai/kg diet; Avian dietary Mallard Duck LC_{50} >5000 mg ai/kg diet; Avian reproduction Bobwhite Quail NOEC ≥1000 mg ai/kg diet; Avian reproduction Mallard Duck NOEC = 500 mg ai/kg diet; Acute toxicity Rainbow Trout 96 hr LC_{50} >87 mg ai/L; Acute toxicity Fathead Minnow 96 hr LC_{50} >94.4 mg ai/L; Chronic toxicity Fathead Minnow 40 day NOEC ≥10.1 mg/L; Acute toxicity Water flea (*Daphnia magna*) 48 hr EC_{50} >100 mg ai/L; Chronic Toxicity Water flea 21 day NOEC ≥10.4 mg/L; Chronic Toxicity Midge (*Chironomus riparius*) 28 day NOEC ≥100 mg/L ; Acute Contact Toxicity Honeybee 48 hr LD_{50} >100 µg ai/bee; Acute Oral Toxicity Honeybee 48 hr LD_{50} >107 µg ai/bee; Acute Toxicity Earthworm (*Eisenia foetida*) 14 d LC_{50} >10,000 mg ai/kg dry soil; Sub-acute Toxicity Earthworm 56 d NOEC ≥1.07 mg ai/kg dry soil; Long-term Impact nitrogen and carbon cycles soil microbial activity 28 d NOEC ≥0.125 mg ai/kg soil; Acute Toxicity Freshwater green algae (*Pseudokirchneriella subcapitata*) 96 h EC_{50} = 0.135 mg ai/L; Acute Toxicity Freshwater blue-green algae (*Anabaena flos-aquae*) 120 h EC_{50} = 11 mg ai/L; Acute Toxicity Saltwater diatom (*Skeletonema costatum*) 120 h EC_{50} = 13.1 mg ai/L; Acute Toxicity Freshwater diatom (*Navicula pelliculosa*) 120 h EC_{50} = 6.8 mg ai/L; Acute Toxicity Duckweed (*Lemna gibba*) 7 d EC_{50} = 0.00257 mg ai/L.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: not included

Analytical Methods: Pyroxsulam identity is determined by liquid chromatography with ultraviolet detection and confirmed by liquid chromatographic mass spectrometry.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry Source(s): Dow AgroSciences

quinclorac

3,7-dichloro-8-quinolinecarboxylic acid

CAS # Acid: 84087-01-4

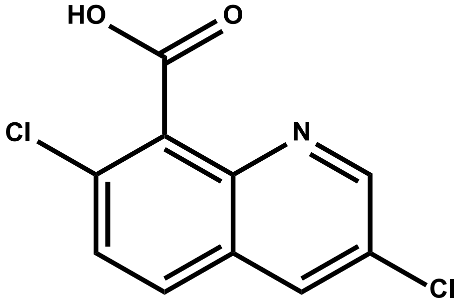
$4^{(O)}$

NOMENCLATURE

Common name: quinclorac (ISO, WSSA)
Other name(s): BAS 514; BAS 51400H; BAS 51405H; BAS 51407H; BAS 51416H; BAS 51434H; BAS 52700H (quinclorac + propanil); BAS 52701H (quinclorac + propanil); 3,7-dichloroquinoline-8-carboxylic acid (IUPAC)
Trade name(s): CLEARPATH®; FACET® 75 DF; FACET® L; PARAMOUNT®; DRIVE®; DRIVE® XLR8; ONETIME®; TRITON® C; BROADHEAD®; Q4® PLUS
Chemical family: quinoline carboxylic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
quinclorac



Molecular formula: $C_{10}H_5Cl_2NO_2$
Molecular weight: 242.06 g/mole
Description: Colorless crystal, faint odor
Density: 0.5 g/mL (technical)
Melting point: 237 C
Boiling point: NA
Vapor pressure: $<1.33 \times 10^{-5}$ Pa
Stability: Stable to heat and light; Stable at pH 3-9
Solubility:
water 62 mg/L (20 C)
organic solvents g/100 mL (25 C):
acetone 0.25
methylene chloride 13.4
pK_a: 4.34 (20 C) (weak acid)
K_{ow}: 0.07 (pH 7)

HERBICIDAL USE

Quinclorac can be applied PRE, delayed PRE, and early POST at 0.28-0.56 kg ai/ha in rice. It controls certain annual grasses such as barnyardgrass and foxtail spp. and also has activity on certain annual and perennial broadleaf weeds such as field bindweed. Quinclorac also can be applied postemergence to turfgrasses for the control of many broadleaf and grass weeds. Additionally, quinclorac is used for weed control in fallow systems, grass grown for seed, preplant wheat, preplant and in-crop sorghum, and noncrop areas.

USE PRECAUTIONS

Fire hazard: FACET is non-flammable.
Corrosiveness: Non-corrosive
Storage stability: 2 yr.
Cleaning glassware/spray equipment: Wash with detergent and water
Emergency exposure: Symptoms of poisoning include general congestive hyperemia.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Not completely understood. In susceptible broadleaves, quinclorac action appears to be similar to that of native auxin (IAA). In susceptible grasses, however, quinclorac may inhibit an enzyme associated with cellulose (cell wall) biosynthesis. Its effect on grasses may also be due to increases in ethylene and cyanide production (3). (more details on page 12)
Symptomology: In certain susceptible broadleafs, symptoms may resemble those of auxin-type herbicides, including mild epinastic bending of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping or curling. This is followed by growth inhibition, chlorosis at the growing points, wilting, and necrosis. In susceptible grasses, rapid chlorosis begins in a band at the zone of elongation in newly expanding leaves (4), followed by general foliar chlorosis and necrosis.
Absorption: Readily absorbed by the emerging grass coleoptile and by roots when soil applied. Absorption of POST-applied quinclorac occurs in Southern crabgrass, Kentucky bluegrass (2), barnyardgrass, and cleavers (1), but may be more limited in certain other species. Quinclorac movement across the plasmalemma probably occurs by ion trapping as with other weak acid herbicides.
Translocation: Readily translocated in both phloem and xylem. Quinclorac applied to the youngest fully expanded leaf of Kentucky bluegrass translocated 28 and 7% to untreated leaves and roots, respectively, by 32 h after application (2).
Metabolism in plants: Quinclorac is slowly metabolized in plants. Less than 4% of applied quinclorac was metabolized after 5 d in tolerant Kentucky bluegrass and susceptible southern crabgrass (2).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: A quinclorac-resistant biotype of smooth crabgrass has developed in California. Resistance appears to be due to an altered site of action involving the cellulose biosynthetic pathway.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: No degradation at 2000 LUX for 7 d.
Other degradation: Degraded microbially.

Persistence: Residues may injure certain susceptible crops planted 1 yr after application.
Mobility: Variable depending on soil characteristics, organic matter and soil percolation rate.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade quinclorac unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >2610 mg/kg; Dermal LD_{50} rabbit, 2000 mg/kg; 4-h Inhalation LC_{50}, NA; Skin irritation rabbit, none; Skin sensitization, NA; Eye irritation rabbit, none

Subchronic toxicity:

90-day dietary, rat: NOEL 302 mg/kg/d (male), 358 mg/kg/d (female); decreased body weight gain, food consumption, increased water intake, increased serum liver enzymes and focal nephritis

21-day dermal, rabbit: NOEL >1000 mg/kg/d; no systemic effects.

Chronic toxicity:

18-month dietary, mouse: NOEL 37.5 mg/kg/d; decreased body weight; not carcinogenic

24-month dietary, rat: NOEL 385 mg/kg/d (males), 478 mg/kg/d (females); decreased body weight (females), increased pancreatic acinar hyperplasia. Not carcinogenic

12-month dietary, dog: NOEL 142 mg/kg/d (males), 140 mg/kg/d (females); reduced body weight, increased liver weight and kidney weight, anemia and kidney degeneration

Teratogenicity:

Rat: NOEL maternal 70 mg/kg/d, developmental >438 mg/kg/d; maternal mortality at high dose, no developmental effects

Rabbit: NOEL maternal 70 mg/kg/d, developmental 200 mg/kg/d; maternal decreased body weight gain and food consumption; development post implantation loss and decreased pup weight.

Reproduction:

Rat: NOEL parental and developmental 200 mg/kg/d, reproductive >600 mg/kg/d. Parental reduced body weight; decreased pup weight, viability and development delays

Mutagenicity:

Gene mutation: Ames test negative; CHO/HGPRT negative

Structural chromosome aberration: Human lymphocyte *in vitro* negative (at non-cytotoxic doses); mouse micronucleus negative

DNA damage/repair: *B. subtilis* REC assay negative; rat hepatocyte UDS assay negative

Wildlife:

Bobwhite quail oral LD_{50}, >2000 mg/kg; Honey bee, non-toxic; Rainbow trout 96-h LC_{50}, >100 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: Quinclorac was synthesized and discovered by BASF and has been developedand commercialized in the U.S. since 1982.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama; Advan; Albaugh/Agri Star; BASF; FMC; Isagro; Nufarm; PBI Gordon

Reference(s):

1. Berghaus and Wuerzer. 1987. Proc. Eur. Weed Res. Soc. Symp. 28:81.
2. Chism, W. J. et al. 1991. Weed Technol. 5:771.
3. Grossman and Kwiatkowski. 1993. J. Plant Physiol. 142:457.
4. Koo, S. J. et al. 1994. Weed Sci. 42:1.

quizalofop-P

(2R)-2-[4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]propanoic acid

CAS # Acid: 94051-08-8
Ethyl ester: 100646-51-3
Tefuryl: 119738-06-6

$1^{(A)}$

NOMENCLATURE

Common name: quizalofop-P (ANSI, BSI, ISO, WSSA) for the R isomer; quizalofop (ANSI, BSI, ISO, WSSA) for the racemic mixture of R and S isomers.

Other name(s): (Acid) (R)-2-[4-(6-chloroquinoxalin-2-yloxy) phenoxy]propionic acid; (Ethyl ester formulation) quizalofop-P-ethyl. The following names all refer to quizalofop ethyl ester: DPX –Y6202; FBC-32197; NC 302; NCI 96683; quinofop-ethyl; quizalofop-ethyl; xylofop-ethyl; ethyl 2-[4-(6-chloro-2-quinoxalinyloxy) phenoxy]propionate; ethyl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy]propionate (IUPAC)

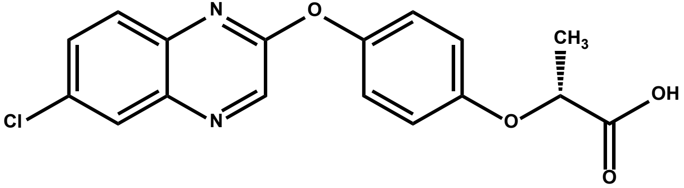
Trade name(s): ASSURE®; TARGA®

Chemical family: aryloxyphenoxy propionate; aryloxyphenoxy propionoic acid

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

quizalofop-P acid



Molecular formula: Acid $C_{17}H_{13}ClN_2O_4$; Ethyl ester $C_{19}H_{17}ClN_2O_4$; Tefuryl $C_{22}H_{21}ClN_2O_5$

Molecular weight: Acid 344.75 g/mole, Ethyl ester 372.81 g/mole; Tefuryl 428.87 g/mole

Description: Colorless crystals

Density: 1.34 g/mL

Melting point: 91.7-92.1 C

Boiling point: 220 C (2.67 x 10^1 Pa)

Vapor pressure: 4.0 x 10^{-5} Pa (20 C)

Stability: Moderately stable to UV light; decomposes at 320 C

Solubility:

water 0.3 mg/L (20 C)
organic solvents g/100 mL (20 C)
acetone 11 hexane 0.26
benzene 29 xylene 12.1

pK_a: 1.25 (weak acid)

K_{ow}: log K_{ow} = 4.66 (23 C)

HERBICIDAL USE

Quizalofop-P provides POST control of annual and perennial grass weeds in soybeans and non-crop areas. It can be applied POST at 35-84 g ai/ha in soybeans, POST at 84-112 g ai/ha in non-crop areas, and POST in a spray-to-wet application at 0.75% v/v for spot treatment in soybeans. Quizalofop-P controls nearly all weedy annual grasses and most perennial grass weeds including johnsongrass, bermudagrass, quackgrass, and wirestem muhly. A nonionic surfactant or crop oil concentrate is required for maximum efficacy.

USE PRECAUTIONS

Fire hazard: The product ASSURE is combustible; flash point is 61 C

Corrosiveness: Mildly corrosive; undiluted product may harm painted surfaces

Storage stability: Stable for 1 yr at (45 C) Do not subject to temperatures below (0 C)

Cleaning glassware/spray equipment: Detergent wash and rinse

Emergency exposure: Flush skin and eyes with large quantities of water for at least 15 min; call a physician. If ingested, do not induce vomiting; Drink large quantities of water. No specific antidote is known. Treat symptomatically.

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details of page 12)

Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop 1-3 wk after application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.

Absorption: Quizalofop-P appears to be rainfast 1 h after field application. The lipophilic nature of quizalofop ethyl ester may facilitate tight binding to the cuticle, thus further reducing the amount reaching leaf cells. Quizalofop-P ester presumably diffuses readily across the plasmalemma. Once inside the cell, the herbicide is rapidly deesterified to quizalofop acid which dissociates in the relatively alkaline cytoplasm. The anion is trapped inside the cell due to its inability to traverse the plasmalemma, a consequence of its negative charge and low lipophilicity. If quizalofop butyl ester hydrolyzed outside the cell, the relatively acid environment allows a significant proportion of quizalofop acid to remain in the protonated (undissociated) from which readily diffuses across the plasmalemma and into the cell. Upon entering the alkaline cytoplasm, the acid dissociates and is trapped inside.

Translocation: Quizalofop-P ethyl ester is systemic and is principally translocated in the symplasm (including the phloem). It accumulates in meristematic regions of the shoot and root, although the rate of translocation is slow.

Mechanism of resistance in plants: Quizalofop-P ethyl ester is hydrolyzed rapidly in plants of quizalofop-P acid. In soybeans and cotton, the quizalofop acid was converted to phenol metabolites or was conjugated to glucose.

BEHAVIOR IN SOIL

Sorption: Quizalofop ethyl ester is moderately adsorbed on sandy loam soils and strongly adsorbed to silt loam soils.

K_{oc}: Average is 510 mL/g for quizalofop ethyl ester (8).

Transformation:Photodegradation: Half-life was 40 d on sandy loam soil.

Other degradation: Rapidly degraded by microbes under aerobic and anaerobic conditions.

Persistence: Moderate residual with an average half-life of 60 d). Quizalofop may suppress grass weeds germinating after a POST application, but degree of suppression or control is related to herbicide rate, soil characteristics, and soil moisture.

Mobility: Very low soil mobility.

Volatilization: NA

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade quizalofop ethyl ester unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 1670 mg/kg, female rat, 1480 mg/kg, male mouse, 2350 mg/kg, female mouse, 2360 mg/kg; Dermal LD_{50} mouse, rat, and rabbit >5000mg/kg; 4-h inhalation LC_{50} rat, 5.8 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

ASSURE: Oral LD_{50} male rat, 6600 mg/kg, female rat, 5700 mg/kg; Dermal LD_{50} rabbit, > 5000 mg/kg; 4-h inhalation LC_{50} rat, > 5 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, severe

Subchronic toxicity:

90-d dietary, rat: NOEL male 40 mg/kg

Chronic toxicity:

18-mo dietary, mouse: NOEL 10 mg/kg; liver effects

24-mo dietary, rat: NOEL 25 mg/kg; not oncogenic; liver effects

12-mo dietary, dog: NOEL 400 mg/kg (highest level tested)

Teratogenicity:

Rat: NOEL 30 mg/kg/d; non teratogenic

Rabbit: NOEL 30 mg/kg/d; non teratogenic

Reproduction:

Rat: NOEL 25 mg/kg in a 2-generation study; liver effects

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: Unspecified test, negative; Mouse micronucleus, negative

DNA damage/repair: SCE, negative

Wildlife:

Mallard duck oral LD_{50}, 2000 mg/kg; LC_{50} bluegill sunfish 96-h LC_{50}, 0.46-2.8 mg/L; rainbow trout 96-h LC50, 10.7 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical Methods: NA

Historical: First registered in the late 1980s in soybeans in the early 1990's in cotton.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection; Gowan; Nissan

.

rimsulfuron

CAS #: 122931-48-0 **2(B)**

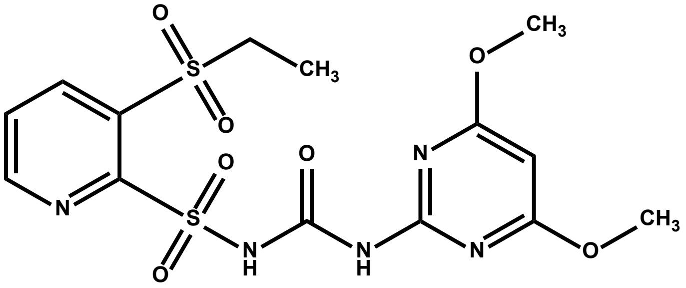
N-[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]-3-(ethylsulfonyl)-2-pyridinesulfonamide

NOMENCLATURE

Common name: rimsulfuron (ANSI, ISO, WSSA)
Other name(s): DPX-E 9636; 1-(4,6-dimethoxypyrimidin-2-yl)-3-(3-ethylsulfonyl-2-pyridylsulfonyl)urea (IUPAC)
Trade name(s): ACCENT GOLD®; BASIS®; BASIS GOLD®; DPX-79406 75DF; PRUVIN™;~~;~~RESOLVE™ DF; SHADEOUT®; STEADFAST®; TRANXIT®; TITUS®
Chemical family: sulfonylurea; pyrimidinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:*rimsulfuron*



Molecular formula: $C_{14}H_{17}N_5O_7S_2$
Molecular weight: 431.44 g/mole
Description: Off-white to tan color, no distinct odor
Density: 0.66 g/mL
Melting point: 176 -178 C
Boiling point: NA
Vapor pressure: 1.5×10^{-6} Pa
Stability: Stable
Solubility:
  water solubility (25 C)
  <10 mg/L unbuffered distilled water
  7,300 mg/L in buffered pH 7.0 water
pK$_a$: 4.1
K$_{ow}$: 0.034 (pH 7, 25 C)

HERBICIDAL USE

Rimsulfuron can be applied early POST to corn and potatoes at 5-15 g ai/ha for the control of many grass and broadleaf weeds in corn and potatoes (1). It is registered for weed control in potatoes in Idaho, Maine, Oregon, Washington, and California. Rimsulfuron is registered for use in corn or in premixtures. Adjuvants such as nonionic surfactant or a crop oil concentrate (COC) play a key role in achieving consistent performance and enhanced activity on certain species. Noxious perennial weeds controlled by rimsulfuron plus surfactant included johnsongrass, quackgrass, sedges, and Canada thistle. Annual *Sorghum* species, foxtails, *Panicum* species, crabgrass, and barnyardgrass are also controlled~~.~~

USE PRECAUTIONS

Fire hazard: Technical and formulated products are dry and non-flammable.
Corrosiveness: Technical and formulated products are non-corrosive.
Storage stability: Technical and formulated products are stable; store product in original container.
Cleaning glassware/spray equipment: Wash lab equipment with water and detergent, then rinse with acetone. Wash spray equipment with water and ammonia at 1% v/v and triple rinse with water. Do not contaminate water, other pesticides, fertilizer, food, or feed in storage.
Incompatibilities: Do not apply with COUNTER 156 insecticide the following spring. Do not tank mix with products containing flumetsulam.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). more details on page 12)
Symptomology: Rapid growth inhibition occurs with POST applications. The initial symptoms of rimsulfuron activity are observed in the meristematic tissues of treated plants. Injury symptoms vary by species and generally included early cessation of growth of sensitive grass and broadleaf species followed by chlorosis, necrosis and plant death (1).
Absorption/translocation: Rapid foliar absorption has been reported following the application of the herbicide in a pH 7 buffer solution. Rimsulfuron moves both in the xylem and phloem.
Metabolism in plants: Crop tolerance to rimsulfuron is based on the differential rate of metabolism of the active compound to inactive metabolites in corn compared to sensitive species. The half-life of rimsulfuron in mature corn leaves was generally about~~o~~ 6 h, whereas in sensitive weed species the half-lives of rimsulfuron were much longer~~.~~
Non-herbicidal biological properties: None identified

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
  Photodegradation: NA
  Other degradation: Rimsulfuron degrades rapidly in soil and water predominantly via chemical pathways. Microbial degradation plays a minor role. Rates of rimsulfuron degradation are influenced by pH. The compound is most stable in neutral soil pH and degrades more rapidly in alkaline and acidic soils. Half-lives in water at 25 C ranged from 4.6 to 0.3 between pH 5.0 and pH 9.0, respectively. The half-life of rimsulfuron in four different soils ranged from 1.7 to 4.3 at 30 C (1, 4).
Persistence: Because of its low use rate and rapid degradation, rimsulfuron is not persistent. No rotational restrictions are expected following application of rimsulfuron at recommended rates in corn.
Mobility: Field studies indicate that rimsulfuron poses very

low risk of leaching into ground water.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade rimsulfuron unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, >5000mg/kg; dermal LD_{50} rabbit, >2000 mg/kg; inhalation 4-h LC_{50} rat, 7.5 mg/L; primary eye irritation rabbit, slightly irritating; dermal irritation rabbit, negative; skin sensitization guinea pig, negative

Subchronic toxicity: NA

Chronic toxicity:
NOEL (2 yr) for male rats 300 mg/kg, female rats 3000 mg/kg; (1 yr) for dogs 50 mg/kg

Teratogenicity: Not teratogenic or oncogenic

Reproduction:
NOEL in 2-generation rat reproduction study 3000 mg/kg

Mutagenicity:
Gene mutation: Ames test, non-mutagenic; CHO, negative

Wildlife:
Bobwhite quail oral LD_{50}, >2250 mg/kg/d; 8-h dietary LC_{50}, >5620 mg/kg; Mallard duck oral LC_{50}, >2250 mg/kg/d; 8-h dietary LC_{50}, >5620 mg/kg; Bluegill sunfish 96-h LC_{50}, >1000 mg/L; Rainbow trout 96-h LC_{50}, >1000 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA **Historical:** Rimsulfuron was discovered in 1989. The herbicide was registered in 1992 for use in corn in Europe. In the US, it was registered for use in potatoes and in corn as a pre-mix with other herbicides in 1995.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Adama**;** DuPont Crop Protection

s-metolachlor

2-chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-[(1*S*)-2-methoxy-1-methyethyl]acetamide

CAS # *S*-metolachlor: 87392-12-9
metolachlor (*R*+*S* isomer): 51218-45-2

$15^{(K_3)}$

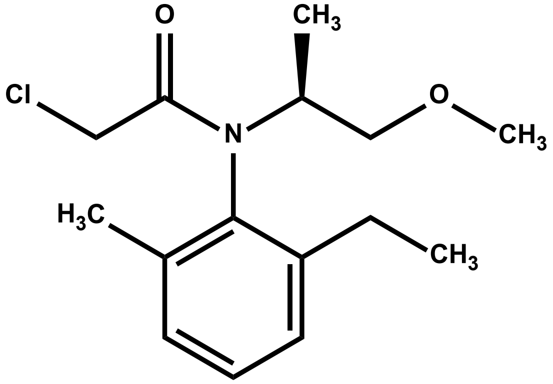
NOMENCLATURE

Common name: *S*-metolachlor (ANSI, BSI, ISO, WSSA)
Other name(s): CGA-77102; mixture of 80–100% 2-chloro-*N*-(6-ethyl-o-tolyl)-*N*-[(1*S*)-2-methoxy-1-methylethyl] acetamide and 20-0% 2-chloro-*N*-(6-ethyl-*o*-tolyl)-*N*-[(1*R*)-2-methoxy-1-methylethyl]acetamide (IUPAC); mixture of 80 – 1000% (*aRS*,1*S*)-2-chloro-6'-ethyl-*N*-(2-methoxy-1-methylethyl)acet-*o*-toluidide and 20 – 0% (*aRS*,1*R*)-2-chloro-6'-ethyl-*N*-(2-methoxy-1-methylethyl)acet-*o*-toluidide (IUPAC)
Trade name(s): BICEP II MAGNUM®; BICEP LITE MAGNUM®; BICEP LITE II MAGNUM®; BICEP LITE II MAGNUM® FC; BOUNDARY® 6.5 EC; CAMIX®; CINCH®; CINCH® ATZ; CINCH® ATZ LITE; DUAL MAGNUM; DUAL II MAGNUM®; DUAL II MAGNUM® SI; DUAL II MAGNUM®; LUMAX®; MEDAL®; MEDAL® II; MEDAL® II AT; ME-TOO-LACHLOR™; ME-TOO-LACHLOR II™; PARALLEL™; PARALLEL PCS; PARALLEL™ PLUS; PARRLAY™; PREFIX™; SEQUENCE®; TRIZMET™ II
Chemical family: acetamide; acetanilide; chloroacetamide; chloroacetanilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

S-metolachlor



Molecular formula: $C_{15}H_{22}ClNO_2$
Molecular weight: 283.80 g/mole
Description: White to tan liquid, odorless
Density: 1.12 g/mL (20 C)
Melting point: -40 C
Boiling point: 282 C (1.013 x 10^5 Pa); 100 C (1.33 x 10^{-1} Pa)
Vapor pressure: 1.73 x 10^{-3} Pa (20 C); 3.73 x 10^{-3} Pa (25 C); 6.53 x 10^{-2} (50 C); 7.06 x 10^{-1} Pa (75 C); 5.46 Pa (100 C); 31.99 Pa (125 C); 159.95 Pa (150 C); Henry's Law constant, 2.4 x 10^{-8} atm m^3/mole (25 C)
Stability: Hydrolyzes at pH 1-9 with a half-life of >200 d (25 C); pH 13 with a half-life of 90 d (20 C)
Solubility:
- water 488 mg/L (20 C)
- organic solvents (25 C):
  - acetone miscible
  - benzene miscible
  - butyl cellusolve miscible
  - cyclohexamone miscible
  - methyl cellusolve miscible
  - dichloromethane miscible
  - propylene glycol insoluble
  - ethanol miscible
  - toluene miscible
  - ethylene glycol insoluble
  - xylene miscible
  - dimethyl formamide miscible
  - ethylene dichloride miscible
  - *n*-hexane miscible
  - *n*-octanol miscible
  - methanol miscible

pK_a: None (non-ionizable)
K_{ow}: 794 (25 C)

HERBICIDAL USE

S-Metolachlor is the result of a proprietary breakthrough in the catalyst system of the manufacturing process for metolachlor. Metolachlor is a 1:1 mixture of *R*- and *S*-isomer pairs (1). The manufacturing process breakthrough allows for selective production of the more active isomer, *S*-metolachlor, in commercial quantities. *S*-Metolachlor is physically and chemically equivalent to metolachlor, but is more active at the site of action in susceptible plants and allows for lower use rates. *S*-Metolachlor has herbicidal utility as follows: early preplant, PPI, PRE, or POST (early POST or at layby) in corn; PPI, PRE, or POST in cotton; PPI, post-plant incorporated, PRE, or POST (at layby) in peanut; PPI or PRE in pod crops; PPI, PRE, or after hilling in potato; PPI or PRE at in safflower; early preplant, PPI, or PRE in grain or forage sorghum (seed-treated with CGA-92194 or CGA-133205 early preplant, PPI, or PRE in soybean; PRE in nursery and landscape plantings; and PRE in certain turfgrass species. *S*-Metolachlor controls yellow nutsedge and many annual grass weeds such as foxtail spp., barnyardgrass, crabgrass spp., fall panicum, signalgrass, witchgrass, and red rice. It also controls certain broadleaf weeds such as redroot pigweed, carpetweed, and Florida pusley. *S*-Metolachlor can be applied through center pivot irrigation systems as well as by conventional ground or air equipment.

It also can be applied in liquid or dry bulk fertilizer. Use rates of *S*-metolachlor are 35% lower than those of the racemic mixture of metolachlor on an active ingredient basis. Sorghum must be treated with Concept or Screen seed treatment to safen the crop from *S*-metolachlor. Certain *S*-metolachlor products contain benoxacor, a safener that protects corn from *S*-metolachlor injury under adverse growing conditions. Benoxacor enhances the glutathione-mediated metabolism of *S*-metolachlor in corn plants. *S*-Metolachlor and benoxacor have similar chemical properties so they behave similarly in the soil profile to provide maximu crop safety.

USE PRECAUTIONS

Fire hazard: Non-flammable

Corrosiveness: Non-corrosive

Storage stability: Stable over several years of storage

Cleaning glassware/spray equipment: Wash with water

Emergency exposure: Dual II Magnum may cause diarrhea, headache, or nausea, usually subsiding within 24 h. If ingested, give 1-2 glasses of water and induce vomiting or lavage stomach. No specific antidote is available, but an aqueous slurry of activated charcoal and a saline cathartic may help.

Incompatibilities: Formulations are compatible with most pesticides and liquid fertilizers. The DUAL II MAGNUM SI formulation was developed specifically for herbicide impregnation on fertilizer.

BEHAVIOR IN PLANTS

Mechanism of action: *S*-metolachlor is a chloroacetanilide herbicide that kills plants by inhibiting very long chain fatty acid biosynthesis (VLFA). (more details on page 14)

Symptomology: Most susceptible weeds fail to emerge from the soil. Injury to grasses presents as malformed and twisted seedlings. Leaves are tightly rolled in the whorl and may not unroll properly. Injured broadleaf weeds have cupped or crinkled leaves with a drawstring or heart shaped appearance.

Absorption/translocation: Absorbed by emerging shoots, especially grass coleoptiles. Some root absorption occurs also. Plants beyond the seedling stage can absorb into roots and translocate to the shoots. *S*-Metolachlor is phytotoxic only to emerging weed seedlings.

Metabolism in plants: Detoxified by cleavage of the methyl ether followed by conjugation with glucose; also detoxified by conjugation of the chloroacetyl group with glutathione (GSH) or; possibly in certain legumes, with homoglutathione. Conjugation probably occurs with a half-life or a few h or less. Involvement of GSH transferase is uncertain. GSH conjugate is subsequently metabolized to the cysteine conjugate, followed by oxidative deamination and reduction to the thiolactic acid conjugate, and oxidation to the sulfoxide derivatives.

Non-herbicidal biological properties: Non known

Mechanism of resistance in weeds: Non specific mode of action is an important factor in preventing the development of weed resistance. No weed resistance related to the use of this mode of action have been observed.

BEHAVIOR IN SOIL

Sorption: Moderately adsorbed to soil. Metolachlor more readily adsorbs to muck or clay soils than to soils with low OM and clay content and more readily adsorbs to OM than to clay.

K_{oc} and K_d: Average K_{oc} is 200 mL/g (3), K_{oc} 66.7 and K_d 1.869 mL/g for a clay with 4.8% OM, 42% clay, and pH 5.9; K_{oc} 21.6 mL/g and K_d 0.108 mL/g for a sand with 0.9% OM, 2.2% clay, and pH 6.5%; K_{oc} 74.4 mL/g and K_d 2.157 mL/g for a sandy loam with 5% OM, 9.2% clay, and pH 5.9; K_{oc} 110.4 mL/g and K_d 0.773 mL/g for a loam with 1.2% OM, 11.2% clay, and pH 7.6.

Transformation:

Photodegradation: Half-life was 70 d in water at 8-45 C and pH 7 with natural light. Half-life was 8 d on sandy loam soil at 15-52 C with natural light. Photodegradation is a major contributor to dissipation in the field, particularly under prolonged lack of rainfall when metolachlor remains on the soil surface.

Other degradation: Half-life was 67 d for aerobic microbial metabolism in sandy loam soil at 25 C in the laboratory, producing [2-ethyl-6-methylphenyl) (2-methoxy-1-methylethyl)amino]oxo-acetic acid as the major metabolite (28% of applied after 90 d); half-life was 81 d for anaerobic microbial metabolism in a sandy loam soil at 25 C producing the same compound as the major metabolite (23% after 29 d). Microbial degradation is a major contributor to field dissipation, especially where metolachlor has moved beneath the soil surface. Non-biological degradation is negligible.

Persistence: Generally provides 10-14 wk of weed control. Residues do not persist long enough to affect crops planted the following season. Field half-life generally is 3-5 mo based on direct metolachlor measurements, but is 30-50 d in northern and 15-25 d in southern areas based on bioassay determinations

Field experiments: Half-lives in bareground dissipation studies sampling o-15 cm: 112 d for sandy loam soil with 0.9% OM and pH 6 in Wisconsin; 97 d for loamy sand with 0.8% OM and pH 6.8 in California; 124 d for silty clay loam with 3.3% OM and pH 6.8 in Iowa.

Mobility: In field-experiments conducted in soybeans grown in Wisconsin, and corn in Iowa and California, no quantifiable metolachlor residues (LOD) = 50 mg/kg) were found below 45 cm. Leaching generally is insignificant when soil OM is >2%.

Volatilization: Generally low, but losses can be significant under certain conditions.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade metolachlor unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 3877 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >4.3 mg/L; Skin irritation rabbit, slight; Skin sensitization, guinea pig

DUAL: Oral LD_{50} male rat, 2500-2690 mg/kg, female rat, 820-1250 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >2.45 mg/L; Skin irritation rabbit, moderate; Eye irritation rabbit, moderate

DUAL 8E: Oral LD_{50} male rat, 2500-2690 mg/kg, female rat, 820-1250 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >2.45 mg/L; Skin irritation rabbit, mild; Eye irritation rabbit, mild

DUAL 25G: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >2.38 mg/L; Skin irritation rabbit, slight; Skin sensitization, guinea pig, no; Eye irritation rabbit, slight

DUAL II: Oral LD_{50} male rat, >2500 mg/kg; female rat, 2114 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat >1.3 mg/L; Skin irritation rabbit, slight;

Skin sensitization guinea pig, no; Eye irritation rabbit, slight

DUAL IIG: Oral LD_{50} rat, >5050 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >4.98 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

BICEP: Oral LD_{50} male rat, >5010 mg/kg; female rat, 4060 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >2.34 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

BICEP II: Oral LD_{50} male rat, 3060 mg/kg; female rat, 1400 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >1.98 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

BICEP LITE: Oral LD_{50} male rat, >5000 mg/kg, female rat, 3030 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LC_{50} rat, >2.73 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

CYCLE: Oral LD_{50} male rat, 2230 mg/kg; female rat, 962 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LD_{50} rat, >1.45 mg/L; Skin irritation rabbit, mild; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

DERBY: Oral LD_{50} rat, 5050 mg/kg; Dermal LD_{50} rabbit, >2020 mg/kg; 4-h inhalation LD_{50} rat, >5.6 mg/L; Skin irritation rabbit, Skin sensitization guinea pig, no; Eye irritation rabbit, mild

PENNANT 5G: Oral LD_{50} rat, >5030 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LD_{50} rat, >3.5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic Toxicity:

90-d dietary, rat: NOEL 90 mg/kg/d (1000 mg/kg); no effects

90-d dietary dog: NOEL 500 mg/kg; no effects

6-mo dietary, dog: NOEL 9.2 mg/kg/d (300 mg/kg); statistically insignificant reduction in body weight gain at ≤ 1000 ppm

21-d dermal, rabbit: NOEL 1000 mg/kg/d (highest dose tested)

Chronic Toxicity: Not carcinogenic at ≤ 3000 mg/kg (highest dose tested); reduced body weight gain at 3000 mg/kg

24 mo-dietary, rat: NOEL 15 mg/kg/d (300 mg/kg); slightly increased incidence of hepatocellular adenomas in females at 3000 mg/kg

12-mo dietary, dog: NOEL 9.2 mg/kg/d (300 mg/kg); reduced body weight gain at 1000 mg/kg

Teratogenicity:

Rat: NOEL maternal 100 mg/kg/d, developmental 300 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 120 mg/kg/d, developmental 360 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 15 mg/kg/d (300 mg/kg); not a reproductive toxin at ≤ 1000 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; Mouse lymphoma, negative

Structural chromosome aberration: Mouse dominant lethal, negative; Chinese hamster/nucleus anomaly, negative; CHO, negative

DNA damage/repair: Rat hepatocytes, negative; Human fibroblasts, negative

Wildlife:

Bobwhite quail oral LD_{50}, 4640 mg/kg/d, 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg/d; 8-d dietary LC_{50}, >10,000 mg/kg; Earthworm LC_{50} in soil, 140 mg/kg; Daphnia 48-h LC_{50}, 25.1 mg/L; Bluegill sunfish 96-h LC_{50}, 10 mg/L; Carp 96-h LC_{50}, 4.9 mg/L; Channel catfish 96-h LC_{50}, 4.9 mg/L; Rainbow trout 96-h LC_{50}, 3.9 mg/L

Use Classification: BICEP products are Restricted use because of ground and surface water concerns with atrazine. CYCLE is Restricted use because of ground and surface water conditions with cyanazine. Other products are General use.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Metolachlor is a mixture of *R*- and *S*- isomer pairs. The isomers identify different spatial arrangements within the molecular structure of metolachlor. Previous metolachlor manufacturing processes resulted in a 50:50 *R*- to *S*-isomer mixture in the final product. Isomers of a product have different levels of biological activity. The majority of the herbicidal activity of metolachlor comes from the *S*-isomer pair. Because it is more active, *S*-metolachlor is used at lower rates than metolachlor. Manufacturing process breakthroughs now allow the selective production of the more active isomer, *S*-metolachlor.

Purification of technical: Vacuum distillation

Analytical methods: Crop residues are extracted by overnight reflux with 6N HCl. After partitioning with organic solvents, samples are cleaned-up by column chromatography. Residues are determined by GC with *N*/*P* electron capture or mass selective. Soil residues are extracted by reflux with 80% methanol. Extracts are partitioned with hexane and cleaned-up on a water-activated alumina column. Parent residues are determined by GC with electron capture or *N*/*P* detection. Water samples are partitioned with dichloromethane and concentration of the organic phase. Residues are determined by GC with *N*/*P* or mass selective detection. Metolachlor is determined in technical samples and formulation by GC using flame ionization detection.

Historical: Metolachlor was synthesized in 1972 by Ciba-Geigy Limited, Basel, Switerland and available commercially for use in corn in 1977. U.S. patent 3,937,730, Belgium patent 800,471, British patents 1,483,311 and 1,438,312. First reported in 1974 (2). *S*-Metolachlor was registered use in the US on March 14, 1997. U.S. Patent 5,002,606.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Adama; Drexel; DuPont Crop Protection; Monsanto; Syngenta Crop Protection

Reference(s):

1. Böger, P., B. Matthes, and J. Schmalfuss. 2000.

Pest Manag. Sci. 56:497-508.
2. Gerber, H.R. 1974. Proc. 12th Br. Weed Control Conf. 2:787.
3. Moser, H., et al. 1983. Proc. 5th IUPAC Pestic. Chem. Congress, 315.
4. Wauchope, R.D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

saflufenacil

CAS# 372137-35-4

14$^{(E)}$

N'-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide

NOMENCLATURE

Common name: saflufenacil

Other names: AC433,379; BAS800H; N′-{2-chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl) pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide (IUPAC)

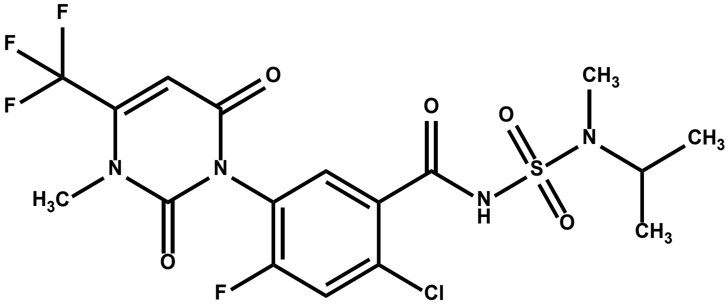
Trade names: HEAT™; DETAIL™; ERAGON®; INTEGRITY®; KIXOR®; OPTILL®; OPTILL® PRO; SHARPEN®; TREEVIX®; VERDICT™

Chemical family: Uracil (pyrimidinedione) amide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

saflufenacil



Molecular formula: $C_{17}H_{17}ClF_4N_4O_5S$

Molecular weight: 500.9 g/mole

Description: Odorless white powder

Density: 1.6 g/mL

Melting point: 189.9 C

Boiling point: NA

Vapor pressure: 2.0×10^{-14} Pa (25 C)

Stability: Stable if stored and handled properly

Solubility:

Water pH 5: 0.003 g/100 mL
pH 7: 0.21 g/100 mL
Acetone 27.5 g/100 mL
Acetonitrile 19.4 g/100 mL
Methanol 2.98 g/100 mL

pK_a: 4.41

K_{ow}: 368.2

HERBICIDAL USE

Saflufenacil is used in the following field and agricultural crops: chickpea, corn, cotton, dry edible beans (harvest aid/desiccation only), English pea, fallow and postharvest, field pea, rice, small grains, sorghum (grain), soybean, sunflower (harvest aid/desiccation only), noncropland areas, citrus, pome fruit, and nut trees. Rates for pre-planting burndown and preemergence applications in row crops range from 18 to 50 g ai/ha depending on crops and countries. Burndown rate for citrus, pome fruit, and nut trees is 25 g ai/ha. POST application to row and tree crops will cause severe crop injury except for harvest aid/desiccation use. Burndown rates for fallow/post harvest treatment and non-cropland area are 25-100 and 25-150 g ai/ha, respectively. Saflufenacil provided control of many broadleaf weeds such as common lambsquarters, marestail, mustards, nightshade, palmer amaranth, redroot pigweed, wild sunflower, and velvetleaf. An adjuvant and fertilizer are required for maximum weed control.

USE PRECAUTIONS

Fire hazard: Not self-igniting, not classified as oxidizing.

Corrosiveness: Corrosive effects to metal are not anticipated.

Storage stability: Avoid temperatures above 40 °C. Changes in the properties of the product may occur if stored above indicated temperature for extended periods of time.

Storage duration: 24 Months

Emergency exposure: Saflufenacil is not harmful after ingestion, dermal exposure or inhalation. It is also not irritating to eyes or skin and is not a sensitizer.

Incompatibilities: Avoid storing saflufenacil with strong oxidizing agents.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox). (more details on page 14)

Symptomology Following inhibition of protoporphyrinogen-oxidase by saflufenacil, plant death is the result of membrane damage. Under active growing conditions, susceptible emerged weeds usually develop chlorotic and necrotic injury symptoms within hours and die within a few days. Susceptible emerging weed seedlings will usually die as they reach the soil surface or shortly after emergence.

Absorption/translocation: Saflufenacil is rapidly absorbed by roots and foliage. Once absorbed, it is predominantly translocated via the xylem, with some movement in the phloem. Low translocation of root-absorbed saflufenacil in corn shoot partially contributes to saflufenacil selectivity in corn

Metabolism in plants: Crop tolerance to saflufenacil is partially due to rapid metabolism. Susceptible weed species metabolize saflufenacil slowly or not at all.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: A codon deletion of the target PPO gene in common waterhemp was reported to confer resistance to lactofen, a protoporphyrinogen oxidase inhibitor. Cross resistance of this biotype to saflufenacil is unknown.

BEHAVIOR IN SOIL

Sorption: K_{oc}= 9 to 56 (6 soils**)**

Transformation: Saflufenacil was found to degrade rapidly in the environment.

Photodegradation:
DT_{50} = 66 days under soil photolysis
DT_{50} = 22 days under aqueous photolysis (pond)
Other degradation:
Hydrolysis stable at pH < 7, half-life 5 days at pH 9

Persistence:
Field persistence: terrestrial dissipation DT_{50} = 1 - 36 days (7 sites); Lab experiments: aerobic metabolism, DT_{50} = 9 - 32 days (4 soils)
Mobility: Mobile to very mobile, hydrophilic.
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.
Acute toxicity:
LD_{50} rat (oral) > 2,000 mg/kg
LC_{50} rat (by inhalation) > 5.3 mg/l 4 h, No mortality was observed, tested as dust aerosol.
LD_{50} rat (dermal) > 2,000 mg/kg
Saflufenacil is not mutagenic, neurotoxic, immunotoxic nor genotoxic.
Short-term, sub-chronic and chronic toxicity studies in rats, mice and dogs identified the hematopoietic system as the target organ of saflufenacil. Protoporphyrinogen oxidase inhibition in the mammalian species may result in disruption of heme synthesis which in turn causes anemia.
Carcinogenicity studies in rats and mice showed no evidence of increased incidence of tumors at the tested doses. Saflufenacil is classified as “not likely carcinogenic to humans.”
Teratogenicity:
Increased fetal susceptibility was observed in the developmental toxicity studies in the rat and rabbit and in the 2-generation reproduction study in the rat.
Wildlife:
Ecotoxicological testing indicates no concerns for acute or chronic effects on birds, fish, aquatic invertebrates, sediment-dwelling organisms, earthworms, honeybees, and other terrestrial invertebrates.

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Multi step integrated process, followed by filtration-washing, recrystallization, drying and packaging.
Purification of technical: purity > 94%
Analytical methods: HPLC reversed-phase method with quantitative UV detection.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry Source(s): BASF
Reference(s):

1. Grossmann, K, R. Niggeweg, N. Christianse, R. Looser, and T. Ehrhardt. 2010. The herbicide saflufenacil (Kixor™) is a new inhibitor of protoporphyrinogen IX oxidase activity. Weed Sci. 58:1-9.
2. Grossmann, K, J. Hutzler, G. Caspar, J. Kwiatkowski, and C. Brommer. 2011. Saflufenacil (Kixor™): biokinetic properties and mechanism of selectivity of a new protoporphyrinogen IX oxidase inhibiting herbicide. Weed Sci. 59:290-298.

siduron

CAS #: 1982-49-6 **$7^{(C_2)}$**

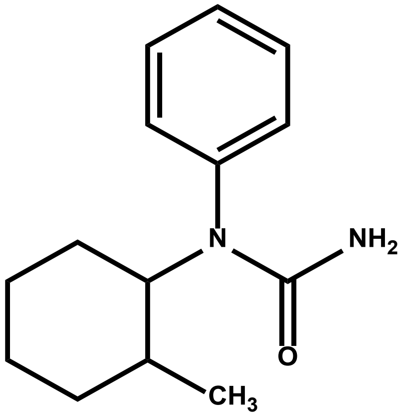
N-(2-methylcyclohexyl)-*N′*-phenylurea

NOMENCLATURE

Common name: siduron (ANSI, BSI, ISO, WSSA)
Other name(s): DuPont 1318; 1-(2-methylcyclohexyl)-3-phenylurea (IUPAC); (2-methylcyclohexyl)-3-phenylurea
Trade name(s): TUPERSAN®
Chemical family: phenylurea; substituted urea; urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
siduron



Molecular formula: $C_{14}H_{20}N_2O$
Molecular weight: 232.33 g/mole
Description: White crystalline solid, odorless
Density: 1.08 g/mL (25 C)
Melting point: 133-138 C
Boiling point: NA
Vapor pressure: 5.3 x 10^{-7} Pa (25 C); <10^{-1} Pa (100 C)
Stability: Stable to UV light
Solubility:
water 18 mg/L (25 C)
organic solvents g/100 mL (25 C):
cellosolve 17.5
dimethylacetamide 36.7
dimethylformamide 26
ethanol 16
isophorone 11.8
methylene chloride 11.8
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 3.8

HERBICIDAL USE

Siduron can be applied PRE at 2.2-6.7 kg ai/ha in-13.4 kg ai/ha in established turf for control of annual grasses such as crabgrass spp., foxtail spp., and barnyardgrass. Siduron can be applied safely in bluegrass, fescue, perennial ryegrass, Zoysia, and certain other species.

USE PRECAUTIONS

Fire hazard: The product TUPERSAN is dry and non-combustible.
Corrosiveness: The product TUPERSAN is non-corrosive.
Storage stability: Stable under normal conditions
Cleaning glassware/spray equipment: Flush equipment with several changes of water after removing nozzle tips and screens (clean these parts separately). Clean glassware by washing with detergent followed by acetone rinse.
Emergency exposure: May irritate eyes, nose, throat, and skin.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Unlike other substituted urea herbicides, siduron is not a potent inhibitor of photosynthesis. Phytotoxic symptoms maybe associated with root growth inhibition (3). (more details on page 13)
Symptomology: NA
Absorption/translocation: Readily absorbed by roots, but not efficiently absorbed into foliage. Siduron readily translocates acropetally in the xylem.
Metabolism in plants: No siduron metabolites were detected in barley after an 8-d absorption period (2)
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Adsorption increases as clay or OM content increases. Siduron adsorption also increases as cation exchange capacity of clay increases. The amount adsorbed on Keyport silt loam in equilibrium with 1 mg/kg in soil solution at 22.5 C is 2.5 mg/kg.
K_{oc}: Average is 420 mL/g (4)
Transformation:
Photodegradation: Negligible losses
Other degradation: Primarily degraded by microbes. Certain soil microbes can utilize siduron as a sole carbon source. Two bacterial and one fungal species capable of metabolizing siduron have been isolated (1)
Persistence: Moderate residual with a typical field half-life of 90 d (4). Siduron residues are undetectable 1 yr after application.
Mobility: Moderately resistant to leaching. Movement is least in soils high in clay or OM and greatest in sand (5).
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade siduron unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, >7500 mg/kg; Dermal LD_{50}, NA; 4-h inhalation $LC_{50,}$ NA; Skin irritation rabbit, none with a 10% suspension, mild with a 25% suspension, moderate-strong with a 40% suspension; Skin sensitization, NA; Eye irritation, NA

Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >10,000 mg/kg; Mallard duck 8-d dietary LC_{50}, >10,000 mg/kg

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: First described as a herbicide by R. W. Varner et al. at the Northeastern Weed Control Conference in 1965.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection; Gowan; PBI Gordon

Reference(s):

1. Belasco and Langsdorf. 1969. J. Agric. Food Chem. 17:1004.
2. Splittstoesser and Hopen. 1968. Weed Sci. 16:305.
3. Splittstoesser and Hopen. 1970. Physiol. Plant. 23:964.
4. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
5. Weed, M. B. et al. 1966. Abstr. Weed Sci. Soc. Am. 75.

sethoxydim

CAS #: 74051-80-2

$1^{(A)}$

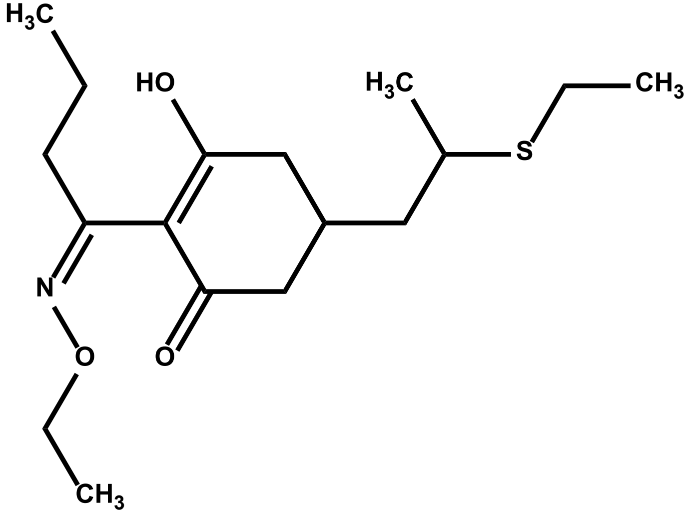
2-[1-(ethoxyimino)butyl]-5-[2-(ethylthio)propyl]-3-hydroxy-2-cyclohexen-1-one

NOMENCLATURE

Common name: sethoxydim (BSI, ISO, WSSA)
Other name(s): BAS 9052 6H; NP-55; (5RS)-2-[(EZ)-1-(ethoxyimino)butyl]-5-[(2RS)-2-(ethylthio)propyl]-3-hydroxycyclohex-2-en-1-one (IUPAC)
Trade name(s): POAST®; POAST® PLUS; POAST® ULTRA; REZULT® G; SEGMENT®
Chemical family: cyclohexanedione; cyclohexane-dione oxime; cyclohexenone; cyclohexene oxime

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
sethoxydim



Molecular formula: $C_{17}H_{29}NO_3S$
Molecular weight: 327.48 g/mole
Description: Amber-colored, oily liquid, odorless
Density: 1.04 g/mL (25 C) (technical)
Melting point: NA
Boiling point: NA
Vapor pressure: $<2.13 \times 10^{-5}$ Pa (25 C)
Stability: Unstable at room temperature
Solubility:
water, 257 mg/L (25 C, pH 5); 4390 mg/L (25 C, pH 7)
organic solvents g/100 mL (20 C):
n-hexane > 1000
methanol > 1000
xylene > 1000
pK_a: 4.16 (25 C) (weak acid)
K_{ow}: 45.1 (pH 7)

HERBICIDAL USE

Sethoxydim controls annual and perennial grasses in several broadleaf crops. It can be applied as follows: POST at 112-448 g ai/ha in soybeans and peanuts; POST at 112-560 g ai/ha in alfalfa, sugar beets, sunflowers, and cotton; POST at 112-560 g ai/ha in flax; as a foliar-applied preplant burndown at 112 g ai/ha for no-till soybeans; POST at 336-560 g ai/ha in many ornamental trees, shrubs, flowers, and ground covers; POST at 1-1.5% v/v as a spray-to-wet application for spot spraying in soybeans and ornamentals; POST at 315 g ai/ha in sethoxydim-resistant field corn. Sethoxydim is also used for control of annual and perennial grass weeds in dry beans; canola; lentils; tobacco; certain vegetable, fruit, and nut crops; specified turf; nonfood; and noncrop areas. An oil adjuvant or nonionic surfactant is required for maximum efficacy.

USE PRECAUTIONS

Fire hazard: The products POAST and POAST PLUS are non-flammable; flash points are 142 C and 141 C, respectively
Corrosiveness: POAST and POAST PLUS are non-corrosive to equipment.
Storage stability: Stable for 2 yrs; POAST should be maintained above 0 C to keep from freezing.
Cleaning glassware/spray equipment: Detergent wash and rinse
Emergency exposure: Wash eyes with water and skin with soap and water; consult a physician if irritation persists. If POAST is ingested, do not induce vomiting; dilute with water and get medical attention.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of of acetyl CoA carboxylase (ACCase). (more details on page 12)
Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Leaf chlorosis and eventually necrosis develop 1-3 wk after application. Leaf sheaths become brown and mushy at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic. With PRE applications, the primary root is inhibited and leaves fail to emerge from coleoptile.
Absorption: Rapidly absorbed into roots or leaves, particularly when applied with an oil adjuvant or other adjuvant. Sexthoxydim generally is rainfast by 1 h after application, although reduced herbicide efficacy has been noted when rainfall occurs 2 h after application (1). Sethoxydim probably moves across the plasmalemma by passive diffusion (6). The relatively acid environment outside the cell presumably allows a significant proportion of sethoxydim to remain in the prontonated (undisscociated) form which readily diffuses across the plasmalemma and into the cell. Once inside the cell, sethoxydim dissociates in the relatively alkaline cytoplasm, trapping the sethoxydim anion inside the cell due to its inability to traverse the plasmalemma, a consequence of its negative charge and low lipophilicity. Thus the ion trapping principles facilitate a build-up of sethoxydim in the symplasm.

Translocation: Sethoxydim is systemic and translocates both in the phloem and xylem, although primarily in the phloem. It accumulates in meristematic areas of shoots and roots, but the rate of translocation out of treated leaves is low and the extent of translocation is limited (5, 10).

Metabolism in plants: Sethoxydim detoxification occurs rapidly in plants, particularly in tolerant grasses. In quackgrass, barnyardgrass, alfalfa, and navy beans, 98% applied sethoxydim was metabolized to at least nine products by 24 h after application (3). Two of these metabolites probably were photodegradation products and one was identifies as desethoxy-sethoxydim.

Non-herbicidal biological properties: Stimulates increased sugar content of sugarcane at harvest.

Mechanism of resistance in plants: Most weed biotypes have developed resistance to aryloxyphenoxy propionates with cross-resistance to the cyclohexanediones appear to have an ACCase that is insensitive to the herbicide. However in diclofop-resistant rigid ryegrass from Australia, cross-resistance to a number of herbicides including sethoxydim, is not due to differential ACCase sensitivity (7). Rather, resistance may be due to increased herbicide metabolism or sequestration away from the site of action.

BEHAVIOR IN SOIL

Sorption: Adsorption varies with OM content.

K_{oc}: Average is 100 mL/g (estimates) at pH 7 (9); loam

K_d: 0.09 mL/g for a sand and 0.68 mL/g for a silt loam

Transformation:

Photodegradation: Photolysis is <1 h in water and <4 h in soil.

Other degradation: Microbially degraded

Persistence: Rapidly degraded with an average field half-life of 5 d

Mobility: NA

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade sethoxydim unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 2676-3124 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50} rat, 6.1 mg/L; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

POAST: Oral LD_{50} rat, 4.1 mg/kg; Dermal LD_{50} rat, >5000 mg/kg; 4-h inhalation LC_{50} rat, > 4.6 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

POAST PLUS: Oral LD_{50} rat, >2200 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, >7.6 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, rat: NOEL NA, LOEL 300 mg/kg

Chronic toxicity:

24-mo dietary, rat: NOEL 18 mg/kg/d; not carcinogenic at up to 162 mg/kg/d

12-mo dietary, dog: NOEL male 8.86 mg/kg/d, female 9.41 mg/kg/d; equivocal anemic effects at doses above the NOEL

Teratogenicity:

Rat: NOAEL maternal 180 mg/kg/d, developmental 650 mg/kg/d; not teratogenic at up to 1000 mg/kg/d

Rabbit: NOAEL maternal 320 mg/kg/d; developmental >400 mg/kg/d; not teratogenic at up to 400 mg/kg/d

Reproduction:

Rat: NOAEL 52.3 mg/kg/d (600 mg/kg)

Mutagenicity: not mutagenic in several tests

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >5620 mg/L; Mallard duck oral LD_{50}, >2510 mg/kg; 8-d dietary LC_{50}, >5620 mg/L; LC_{50} bluegill sunfish 96-h LC_{50}, 100 mg/L; Rainbow trout 96-h LC_{50}, 32 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Confidential

Purification of technical: NA

Analytical Methods: NA

Historical: Sethoxydim was synthesized and discovered by Nippon Soda Co., LTD (Japan) and was developed by BASF in the U.S. where it was first tested in 1978 as BAS 9052 OH.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF; Nufarm

Reference(s):

1. Bryson, C.T. 1988. Weed Sci. 35:115.
2. Burton, J. D. et al. 1989. Pestic. Biochem. Physiol. 34:76.
3. Campbell and Penner. 1985 Weed Sci. 33:771
4. Focke and Lichtenhaler. 1987 Z. Naturforsch. 42c:1361
5. Harker and Dekker. 1982. Proc. N. Cent. Weed Control Conf. 38:37.
6. Hosaka, H. and M. Takagi. 1987. Weed Sci. 35:619.
7. Powles, S. B. et al. 1990. Pages 394-406 in M.B. Green , H.M. LeBaron, and W. K. Moberg, eds., Managing Resistance to Agrochemicals. Am. Chem. Soc. Symp. Ser. 421, Washington DC.
8. Stolenberg, D. E. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
9. Wauchope, R. D. etal. 1992. Rev. Environ. Contam. Toxicol. 123:1.
10. Wills, G.D. 1984. Weed Sci. 32:20.

simazine

6-chloro-*N*,*N*′-diethyl-1,3,5-triazine-2,4-diamine

CAS #: 122-34-9

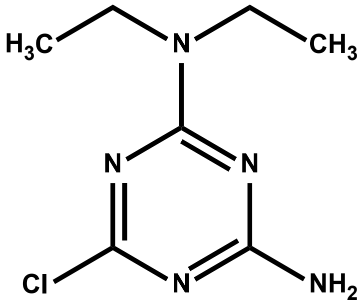
$5^{(C_1)}$

NOMENCLATURE

Common name: simazine (ANSI, BSI, ISO, WSSA)
Other names: G-27692; 2-chloro-4,6-bis(ethylamino)-*s*-triazine; 2-chloro-4,6-bis(ethylamino)-1,3,5-triazine; 6-chloro-N^2,N^4-diethyl-1,3,5-triazine-2,4-diamine (IUPAC)
Trade name(s): AQUAZINE®; CEKUSIMA; FRAMED; PRINCEP®; GESATOP®; SIMTROL; SIMADEX; TOTAZINA
Chemical family: chloro-*s*-triazine; chlorotriazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
simazine



Molecular formula: $C_7H_{12}ClN_5$
Molecular weight: 201.66 g/mole
Description: White, crystalline
Density: 0.436 g/mL (20 C)
Melting point: 225-227 C
Boiling point: NA
Vapor pressure: 1.2×10^{-7} Pa (10 C); 8.1×10^{-7} Pa (20 C); 2.9×10^{-6} Pa (25 C); 4.8×10^{-6} Pa (30 C); 1.9×10^{-4} Pa (50 C); 6×10^{-6} Pa (75 C); 1.3×10^{-1} Pa (100 C); 2 Pa (125 C); 20 Pa (150 C); Henry's Law constant, 9.48×10^{-10} atm m^3/mole
Stability: Decomposed by UV light; slowly hydrolyzed at neutral pH and 70 C, but hydrolysis rate increases at higher or lower pH
Solubility:
water 2 mg/L (0 C); 3.5 mg/L (20 C); 6.2 mg/L (22C); 84 mg/L (85 C)
organic solvents g/100 mL (20 C):
acetone 0.18
chloroform 0.09
ethanol 0.064
ethyl acetate 0.12
n-hexane 0.00066
methanol 0.04
n-octanol 0.051
n-pentane 0.0003 (25 C)
petroleum ether 0.0002
toluene 0.018
pK_a: 1.62 (weak base)
K_{ow}: 122 (25 C)

HERBICIDAL USE

Simazine can be soil-applied preemergence as follows: at 1.1 kg ai/ha in strawberries; at 1.1-2.2 kg ai/ha in almonds and nectarines; at 2.2-4.5 kg ai/ha in apples, avocados, blueberries, caneberries, cranberries, established Christmas trees, filberts, lemons, macadamia nuts, olives, pears, pecans, shelterbelts, sour cherries, and walnuts; at 1.8-4.5 kg ai/ha in peaches, plums, and sweet cherries; at 1.8-4.5 kg ai/ha in lemons; at 4.5-8.9 kg ai/ha in oranges and grapefruit; and at 2.2-5.4 kg ai/ha in grapes. Simazine can also be applied early preplant or PRE at 2.2-4.5 kg ai/ha in corn. It controls many broadleaf and grass weeds including morningglory spp., lambsquarters, nightshade spp., pigweed spp., ragweed spp., smartweed spp., wild mustard, barnyardgrass, crabgrass spp., fall panicum, foxtail spp., witchgrass, and others.

USE PRECAUTIONS

Fire hazard: The products PRINCEP LIQUID and PRINCEP 4L are non-flammable; flash points are >93 C. Simazine technical has low electrical conductivity, but presents a dust explosion hazard.
Corrosiveness: Technical and all formulated products are non-corrosive.
Storage stability: Stable over several years of dry storage.
Cleaning glassware/spray equipment: Wash with water and detergent. If a film builds up in the spray tank due to use of EC formulations, clean with strong detergent or organic solvent.
Emergency exposure: Slight eye, skin, or upper respiratory irritation may occur. If ingested, drink 1-2 glasses of water and induce vomiting or lavage stomach. No specific antidote is available, but ingestion of an aqueous suspension of activated charcoal may help inactivate simazine.
Incompatibilities: Compatible with most other pesticides and fertilizers.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Initial symptoms include interveinal chlorosis of the leaves and yellowing of their margins, followed in susceptible plants by general foliar chlorosis and necrosis. Browning of the leaf tips can occur. Older leaves are more injured than new growth. Root growth is not affected.
Absorption/translocation: Readily absorbed through roots from soil applications and translocated to shoots primarily through the xylem; poorly absorbed into leaves from POST applications. Simazine shows little to no basipetal translocation from the leaves.
Metabolism in plants: Benzoxazinone (DIMBOA)-catalyzed hydrolysis, producing hydroxy simazine, occurs in roots of some tolerant species such as corn and contributes substantially to detoxication for soil-applied simazine. Glutathione conjugation is a major detoxication reaction in certain highly-tolerant species such as corn. *N*-dealkylation of side chains occurs at moderate rates in most plant species, contributing significantly to detoxication only in susceptible

or moderately susceptible species lacking appreciable rates of hydrolysis.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Many species worldwide have developed triazine-resistant biotypes. Most have been selected by continuous use of atrazine or simazine, but are also resistant to other triazines. Those studied at the genetic level have an altered *psbA* gene coding for a glycine in place of a serine on the D1 protein on which the triazine binding site is located. Thus, triazines cannot bind efficiently to the D1 protein and do not block photosynthetic electron transport.

BEHAVIOR IN SOIL

Sorption: More readily adsorbed on muck or clay soils than to soils low in OM and clay

K_{oc} and K_d: Average K_{oc} is 130 mL/g (1). K_{oc} 152 mL/g and K_d 4.31 mL/g for a clay with 4.8% OM, 42% clay, and pH 5.9; K_{oc} 123 mL/g and K_d 0.65 mL/g for a sand with 0.9% OM, 2.2% clay, and pH 6.5; K_{oc} 114 mL/g and K_d 1.27 mL/g for a sandy loam with 1.9% OM, 16.8% clay, and pH 7.5; K_{oc} 103 mL/g and K_d 0.48 mL/g for a loam with 0.8% OM, 9% clay, and pH 6.7

Transformation:

Photodegradation: Stable in water (pH 7, 25 C) under a xenon arc light. Half-life was 21 d on a sandy loam at 25 C under natural light, producing low levels of the mono-*N*-deethylated metabolite (6-chloro-*N*-ethyl-1,3,5-triazine-2,4-diamine), the di-*N*-deethylated metabolite (6-chloro-1,3,5-triazine-2,4-diamine), and hydroxy simazine [4,6-bis(ethylamino)-1,3,5-triazin-2(1*H*)-one] 207 h after application; moderate contribution to dissipation in the field, particularly under prolonged lack of rainfall when simazine remains on the soil surface.

Other degradation: Half-life was 91 d for aerobic microbial metabolism in a sandy loam at 25 C, producing hydroxy simazine as the major metabolite after 1 yr. Half-life was 10-11 wk for anaerobic microbial metabolism in a sandy loam at 25 C. Microbial reactions are the major contributors to dissipation in the field in high pH soils where hydrolysis rates are slow. At low pH, biological degradation is less important because of faster rates of non-microbial hydrolysis producing hydroxy simazine.

Persistence: Average half-life for simazine in ponds is 30 d, but this varies with many factors including the level of algae and weed infestation. On terrestrial sites, simazine has moderate residual with an average field half-life of 60 d (1). On high pH soils, simazine persists longer and residues can injure susceptible crops planted 1 yr after application.

Field experiments: Half-lives in bare ground dissipation studies sampling 0-15 cm: 149 d for a sandy loam with 1.3% OM and pH 7.3 in California; 60 d for a sand with 0.9% OM and pH 7.8 in Florida; 55 d for a loam with 2.1% OM and pH 5.5 in Missouri; 186 d for a loam with 6.2% OM and pH 7.9 in Minnesota.

Mobility: Limited leaching potential under field conditions

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade simazine unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >3100 mg/kg; 4-h inhalation LC_{50} rat, >5.5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

AQUAZINE 90 WDG and PRINCEP CALIBER 90: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >2.4 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

PRINCEP 4L: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2500 mg/kg; 4-h inhalation LC_{50} rat, >9.8 mg/L; Skin irritation rabbit, slight; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, rat: NOEL 200 mg/kg; kidney effects and reduced body weights, with secondary hematopoietic changes at 2000 and 4000 mg/kg

90-d dietary, dog: NOEL 6.7 mg/kg/d; reduced body weights, with secondary hematopoietic changes at 2000 and 4000 mg/kg

21-d dermal, rabbit: NOEL 1000 mg/kg/d (highest dose tested).

Chronic toxicity:

18-mo dietary, mouse: NOEL 5.7 mg/kg/d; not carcinogenic at ≤4000 mg/kg; reduced body weights with secondary decreases in red blood cells, hemoglobin, and hematocrit at ≥1000 mg/kg

24-mo dietary, rat: NOEL 0.5 mg/kg/d; increased incidence of mammary gland carcinoma in females and reduced body weights at ≥100 mg/kg

12-mo dietary, dog: NOEL 0.7 mg/kg/d; hematopoietic and body weight effects at 100 and 1250 mg/kg

Teratogenicity:

Rat: NOEL 10 mg/kg/d; not teratogenic

Rabbit: NOEL 5 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL maternal 10 mg/kg, developmental 500 mg/kg; reduced body weights in dams at ≥100 mg/kg; not a reproductive toxin at ≤500 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative**Structural chromosome aberration:** Chinese hamster/nucleus anomaly, negative; Human lymphocytes, negative

DNA damage/repair: Rat hepatocytes, negative; Human fibroblasts, negative

Wildlife:

Bobwhite quail oral LD_{50}, 1785 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >4640 mg/kg; 8-d dietary LC_{50}, >10,000 mg/kg; Earthworm LC_{50} in soil, >1000 mg/kg; Daphnia 48-h LC_{50}, >100 mg/L; Bluegill sunfish 96-h LC_{50}, >32 mg/L; Rainbow trout 96-h LC_{50}, 70.5 mg/L; Oyster 96-h LC_{50}, >3.7 mg/L

AQUAZINE 80W: Rainbow trout 96-h LC_{50} ,782 mg/L.

Use classification: General use for most products

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Successive *N*-alkylation of cyanuric chloride

Purification of technical: Recrystallization from lower alcohols

Analytical methods: Crop samples are extracted by reflux in 80% acetonitrile, partitioned into ethyl acetate/hexane, and cleaned-up on an Alumina B SepPak. Soil samples are extracted with 80% acetonitrile, partitioned into dichloromethane, and cleaned-up on a water-deactivated alumina column. Crop or soil extracts are analyzed by GC with N/P detection. Water samples are partitioned with dichloromethane, the organic phase is concentrated, and residues are determined by GC with N/P or mass selective detection. Simazine is determined in technical samples and in formulated products using GC with flame ionization detection.

Historical: Synthesis and testing of triazine compounds as herbicides began in 1952 in the Geigy laboratories in Basel, Switzerland. Simazine was first released for experiment station evaluation in 1956 and became commercially available for use in corn in 1958.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Agriliance; Drexel; Syngenta Crop Protection; UAP-Loveland Products; United Suppliers

Reference(s):

1. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

simetryn

CAS #: 1014-70-6

5$^{(C_1)}$

N,N′-diethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: simetryn (ISO, BSI, WSSA)

Other name(s): simetryne; G-32911; N^2,N^4-diethyl-6-methylthio-1,3,5-triazine-2,4-diamine (IUPAC)

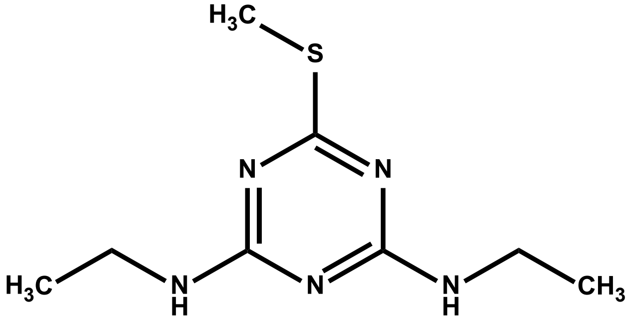
Trade name(s): GYBON

Chemical family: triazine; *s*-triazine; methylthio-*s*-triazine; methylthio triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

simetryn



Molecular formula: $C_8H_{15}N_5S$

Molecular weight: 213.3 g/mole

Description: Solid

Density: 1.02 g/mole

Melting point: 82-83 C

Boiling point: NA

Vapor pressure: 9.4 x 10^{-5} Pa (20 C)

Stability: Stable in neutral, weakly acidic, and weakly alkaline media; hydrolyzed by strong acids and alkalis to 6-hydroxy derivative

Solubility: In water, 400 mg/L (20 C), acetone 400 mg/L, methanol 380 mg/L, toluene 300 mg/L, hexane 4 mg/L

pK_a: 11 (weak base)

K_{ow}: log K_{ow} = 2.8

HERBICIDAL USE

Used in combination with thiobencarb to control broadleaf weeds in rice. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: NA.

Storage stability: NA

Emergency exposure: Eyes or skin; wash with plenty of water

Incompatibilities: Reacts with strong acid or alkaline materials

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)

Symptomology: Chlorosis followed by necrosisof affected tissue.

Absorption/translocation: Absorbed by roots and leaves; translocated primarily in the xylem

Metabolism in plants: NA

Mechanism of resistance in weeds: Altered site of action

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 32-218 mL/g

K_d: 0.37-0.85 mL/g

Persistence:

Field experiments: DT_{50} 309 – 1123 d

Volatilization: Moderately volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade simetryn unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 750-1195 mg/kg; Dermal LD_{50} rat, >3200 mg/kg; Skin or eye irritant rabbit, no

Chronic toxicity:

24-mo dietary, mouse: NOEL 56 mg/kg/d

2-yr, dog dietary: NOEL 10.5 mg/kg/d

Wildlife:

Trout LC_{50} (96 h), 7 mg/L, guppy, 5.2 mg/L; non-toxic to bees; toxic to algae

Use classification: WHO Class III- slightly hazardous

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): NA; Multiple Asian manufacturers; Not sold in U.S.

sodium chlorate

sodium chlorate

CAS #: 7775-09-9

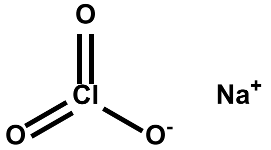
NC

NOMENCLATURE

Common name: sodium chlorate (WSSA)
Other name(s): NA
Trade name(s): ALTACIDE; BARE GROUND BD; BARESPOT® MONOBAR-CHLORATE; BARESPOT UREABOR; BARESPOT WEED & GRASS; BOROCIL IV; CHLORACIL; 3LB CHLORATE DEFOLIANT DESICCANT; DEFOL 6; DROP-LEAF; FALL; HIBAR C; KLOREX; KUSATOL; LEAFEX 2; PRAMITOL® 5PS; PROMETON 5PS; STAA-FREE; RASIKAL; SHED-A-LEAF; TOTAL™; TUMBLEAF
Chemical family: None generally accepted

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
sodium chlorate



Molecular formula: $ClNaO_3$
Molecular weight: 106.44 g/mole
Description: Pale yellow to white crystals, salty taste, odorless.
Density: 2.49 g/mL (15 C)
Melting point: 248 C
Boiling point: Decomposes
Vapor pressure: Essentially zero
Stability: Stable
Solubility:
water, 1,000,000 mg/L (20 C), and 2,300,000 mg/L (100 C)
alcohol soluble
pK_a: NA
K_{ow}: NA

HERBICIDAL USE

Sodium chlorate can be applied as a preharvest desiccant in cotton and certain other crops, in mixture with other herbicides as a soil-sterilant treatment, and for general weed control (including trees and stumps) on non-crop land. Application rates range from 1.68-6.72 kg ai/ha.

USE PRECAUTIONS

Fire hazard: Sodium chlorate is a strong oxidant; contact with combustible materials may cause fire. Clothing and vegetation contaminated with chlorate or its solutions are dangerously flammable. DEFOL 6 is nonflammable; flash point is >93 C.
Corrosiveness: NA
Storage stability: Stable at normal temperatures and when kept isolated from other materials.
Cleaning glassware/spray equipment: Flush with water.
Emergency exposure: If ingested, induce vomiting immediately after drinking 2 glasses of water; repeat until vomit is clear. Wash eyes promptly with warm water for at least 15 min.

BEHAVIOR IN PLANTS

Mechanism of action: In animal systems, sodium chlorate inhibits activity of ATP-sulfurylase, the first enzyme in the biosynthesis of PAPS (3′-phosphoadenosine 5′-phosphosulfate) which is the ubiquitous co-substrate for sulfation (2). Sodium chlorate is a strong oxidizing agent in plants, and also may act to block protein sulfation.
Symptomology: Sodium chlorate applied POST produces brown desiccated foliage.
Absorption/translocation: Readily absorbed into foliage and roots. Little is known of sodium chlorate translocation.
Metabolism in plants: Sodium chlorate is bioactivated to the highly phytotoxic chlorite ion by the reducing activity of nitrate reductase. Further details are unknown.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 10 mg/L (estimated) (1)
Transformation: NA**Persistence:** Average field half-life is estimated at 200 d (1)
Mobility: NA
Volatilization: No losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade sodium chlorate unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 5000 mg/kg; Dermal LD_{50} rabbit, 500 mg/kg; 4-h inhalation LC_{50}, NA; Skin irritation, NA; Skin sensitization, NA; Eye irritation, NA
Subchronic toxicity: NA
Chronic toxicity: NA
Teratogenicity: NA
Reproduction: NA
Mutagenicity: NA
Wildlife: NA
Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: For macro analysis use Methods Clearing House Method 330.0; National Formulary IX. p. 398 (1950).

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Drexel; Cenex/Land O'Lakes; Helena; J. R. Simplot; UAP-Platte; Pro-Serve; Riverside/Terra

Reference(s):

1. Augustijn-Beckers, P. W. M. et al. 1994. Rev. Environ. Contam. Toxicol. 137:1.
2. Baeuerle and Huttner. 1986. Biochem. Biophys. Res. Commun. 141:870.

sulcotrione

CAS #: 99105-77-8

$27^{(F_2)}$

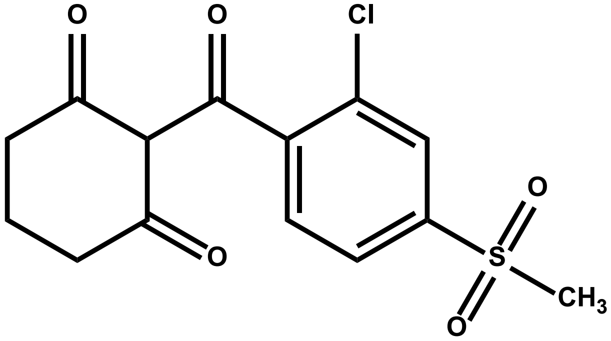
2-[2-chloro-(4-methylsulfonyl)benzoyl]-1,3-cyclohexanedione

NOMENCLATURE

Common name: sulcotrione
Other name(s): ICI-A0051; SC-0051
Trade name(s): MIKADO®
Chemical Family: benzoylcyclohexanedione; triketone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: *sulcotrione*



Molecular formula: $C_{14}H_{13}ClO_5S$
Molecular weight: 328.77 g/mole
Description: Light tan solid
Density: NA
Melting point: NA
Vapor pressure: 5.33×10^{-6} Pa
Stability: Stable in water with or without exposure to sunlight and thermostable up to (80 C)
Solubility:
water 164 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone chlorobenzene.
pK$_a$: None (non-ionizable)
K$_{ow}$: log K_{ow} = < 0

HERBICIDAL USE

Sulcotrione can be applied PRE and POST at 0.25 to 1 kg ai/ha in corn (1, 2, 4). It selectively controls certain annual broadleaf and grass weeds such as large crabgrass, barnyardgrass, fall panicum, lambsquarters, pigweeds, and grasses such as foxtails and *Festuca* species (1). Other crops exhibiting tolerance to this herbicide include sugarcane and winter cereals.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Formulated products are non-corrosive.
Storage stability: Good stability; store in cool, dry place and avoid excess heat; store in original containers only; keep out of reach of children and animals
Cleaning glassware/spray equipment: Clean glassware and equipment with a solution of soap and water; avoid contamination of water by cleaning of equipment or disposal of wastes
Emergency exposure: NA
Incompatibilities: Sulcotrione has been found to be physically compatible with most commercially available herbicides.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme 4-hydroxyphenyl-pyruvate dioxygenase (4-HPPD) affecting carotenoid biosynthesis (more details on page 15)
Symptomology: Treated plants show bleaching symptoms but complete kill is progressive (1).
Absorption/translocation: Sulcotrione is active mostly as a foliar herbicide but additional efficacy is provided through root uptake (1). This residual soil activity gives sulcotrione a clear advantage over herbicides which only have POST activity. This additional efficacy is an important factor for the control of certain weeds such as pigweeds.
Metabolism in plants: Details are not available. Sulcotrione is generally safe to corn up to 900 g ai/ha and no varietal susceptibility has been observed. Under poor growing conditions, however, corn plants may show some foliar discoloration. However, these symptoms are transient and further growth and yield of maize is not affected (1).
Mechanism of resistance in weeds: Development of weed resistance to this herbicide has not been observed.

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation: Sulcotrione is not susceptible to photodecomposition or volatility following application to soil.
Other degradation: Degradation in soil is rapid with half-lives ranging from 15 d in a loamy sand from Toulouse to 72 d in a fine loam from Iowa. The soil degradation of sulcotrione is mainly microbial and no adverse effects, even at very high rates of use, have been observed on soil microorganisms.
Persistence: Sulcotrione is not very persistent in soils. No injury symptoms have been identified in the following crops within a normal rotation: winter wheat, winter barley, winter oil seed rape, potatoes, sugar beet, corn, peas, and beans. If a treated crop is abandoned, corn may be re-seeded but soybean and *Phaseolus* beans must be avoided, even after plowing (1).
Mobility: NA
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade sulcotrione unless otherwise indicated.
Acute toxicity:
This herbicide has a low acute toxicity to mammals

through oral, dermal or inhalation routes. Good user protection is afforded by the very low rate of absorption through skin. Sulcotrione is not a skin sensitizer, not a skin irritant, but it can slightly irritate eyes. Specific LD_{50}, or other data are not available (1).

Chronic toxicity: NA

Teratogenicity:

Rat oral teratology: Non-teratogenic

Mutagenicity:

No genotoxicity was observed *in vivo* (1)

Wildlife:

Sulcotrione has a low toxicity to wildlife including birds (*Anas platyrynchos* and *Colinua virginianua*); fish (*Cyprinus carpio* and *Salmo gairdneri*); daphnia and bees, following both topical and oral application (1).

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: The herbicidal properties of sulcotrione and other triketones were discovered at the Western Research Center of Zeneca Ag Products in 1986. Sulcotrione was divested upon the formation of Syngenta.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Bayer CropScience

Reference(s):

1. Beraud, J.M. et al. 1991. Proc. Brighton Crop Prot. Conf. – Weeds, pp. 51-56.
2. Wilson, J.S. and C.L. Foy. 1990. Weed Technol. 4:731.
3. Mayonado, D.J. et al. 1989. Pestic. Biochem. Physiol. 35:138.
4. Prisbylla, M.P. et al. 1993. Proc. Brighton Crop Prot. Conf. – Weeds, pp. 731-738.

sulfentrazone

CAS #: 122836-35-5

14$^{(E)}$

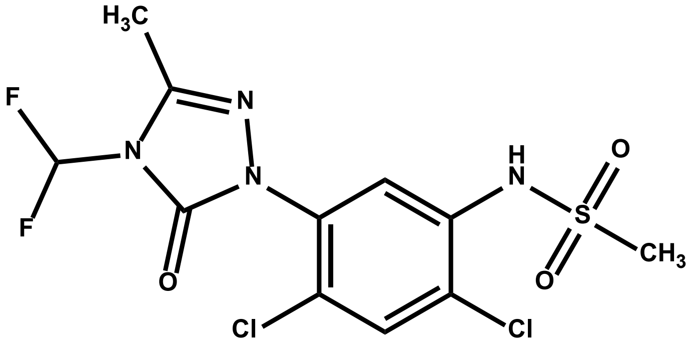
N-[2,4-dichloro-5-[4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl]phenyl]methanesulfonamide

NOMENCLATURE

Common name: sulfentrazone (ISO, WSSA)
Other name(s): F6285; FMC 97285; $2^1,4^1$-dichloro-5^1-(4-difluoromethyl-4,5-dihydro-3-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl)methanesulfonanilide (IUPAC)
Trade Name(s): AUTHORITY™; BORAL™; SPARTAN™
Chemical family: aryl triazinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
sulfentrazone



Molecular formula: $C_{11}H_{10}Cl_2F_2N_4O_3S$
Molecular weight: 387.19 g/mole
Description: Tan solid
Density: 0.53 g/mL (20 C)
Melting point: 121-123 C
Boiling point: NA
Vapor pressure: 1.07 x 10^{-7} Pa (25 C); 1.33 x 10^{-7} Pa (25 C) (1)
Stability: Stable at room temperature
Solubility: 110 mg/L (pH 6); 780 mg/L (pH 7); 1600 pH 7.5
pK_a: 6.56
K_{ow}: 9.8 (pH 7)

HERBICIDAL USE

Sulfentrazone is a soil-applied, pre-emergent herbicide which can be applied either PPI or PRE. Sulfentrazone can be applied at 0.14-0.42 kg ai/ha in soybean and tobacco. Sulfentrazone is also applied at 0.1-0.28 kg ai/ha on sunflower and 0.42 kg ai/ha on sugarcane under SLN registrations in a number of states. Sulfentrazone applied to 0.084-0.28 kg ai/ha on peanut is pending registration. Sulfentrazone is registered under various state labels on several vegetable crops. Sulfentrazone is also registered for use on several turfgrass species.

USE PRECAUTIONS

Fire hazard: Technical and formulated sulfentrazone are non-flammable; flash point is > 100 C.
Corrosiveness: Formulated products are non-corrosive.
Storage stability: Good stability. Store in cool, dry place and avoid excess heat. Store in original containers only. Keep out of reach of children and animals. Do not contaminate water, food or feed by storage or disposal.
Cleaning glassware/spray equipment: Clean glassware and equipment with a solution of soap and water; avoid contamination of water by cleaning of equipment or disposal of wastes. Large spills should be covered to prevent dispersal.
Emergency exposure: If ingested, drink 1-2 glasses of water. Do not induce vomiting or give anything by mouth to an unconscious individual. Contact a medical doctor. If inhaled, expose to fresh air. If breathing discomfort occurs, contact a medical doctor. For skin and eye exposure wash with plenty of soap and water or flush with water for at least 15 minutes, respectively. If irritation occurs or persists get medical attention.
Incompatibilities: Sulfentrazone has been found to be physically compatible with most commercially available herbicides.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme protoporphyrinogen oxidase (PPG or Protox) (more details on page 14)
Symptomology: Susceptible plants emerging from soils treated with sulfentrazone turn necrotic and die shortly after exposure to light. Foliar contact results in rapid desiccation and necrosis of exposed plant tissues. The majority of soybean, tobacco, sunflower, and peanut cultivars have shown no adverse effects when treated with recommended rates of sulfentrazone. However, under cool, wet conditions, at or immediately after application, minor and short-lived effects, such as stunting, and discoloration, have been observed. These effects have not been demonstrated to affect yields.
Absorption/translocation: Sulfentrazone is taken up by the roots and foliage of treated plants. Shoot-root soil placement studies indicate that sulfentrazone is absorbed primarily by the roots of treated plants following soil applications. Symplastic phloem movement is assumed to be limited, because of the rapid foliar desiccation caused by this herbicide.
Metabolism in plants: Sulfentrazone is rapidly metabolized in soybeans leading to a number of metabolic transformations. The major pathway involves oxidative hydroxylation of the methyl group of the triazole ring, followed by further oxidation of the hydroxymethyl function to form a carboxylic function, which is eventually decarboxylated. A secondary pathway involves cleavage of the methanesulfonamide function of the phenyl ring.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Development of weed resistance to this herbicide has not been observed.

BEHAVIOR IN SOIL

Sorption:

K_{oc} = 43 mL/g; K_d < 1 mL/g (1). Low to intermediate sorption

Transformation:

Photodegradation: Sulfentrazone is not susceptible to photodecomposition or volatility following application to soil.

loss of sulfentrazone in soil appears to be primarily by microbial degradation.

Persistence: Results of sulfentrazone field dissipation studies indicate its half-life ranged form 121 to 302 d. The DT_{50} is 32 d. The rotational tolerance of selected crops, based on phytoxicity in field rotation, follow-crop studies, has shown that wheat, barley, rye, oats, triticale can be planted after 3 mo; field corn (including grain, silage, popcorn and seed corn), rice, and sorghum can be planted after 10 mo; cereal grains (buckwheat, pearl millet, proso millet, teosinte and wild rice) and sweet potatoes can be planted after 12 mo; cotton and sweet corn can be planted after 18 mo; and canola and sugarbeets can be planted after 24 mo.

Mobility: Sulfentrazone is moderately mobile in the soil. Mobility is greater than that of alachlor, but less than that of metribuzin.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade sulfentrazone unless otherwise indicated

Acute Toxicity:

Oral LD_{50} rat, 2689 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h Inhalation LC_{50} rat, >4.13 mg/L; Primary eye irritation rabbit, mild; Skin irritation rabbit, none; Skin sensitization guinea pig, negative

4 F formulation: Oral LD_{50} rat, 2084 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h Inhalation LC_{50} rat, >2.72 mg/L; Primary eye irritation rabbit, none; Skin irritation rabbit, slight; Skin sensitization guinea pig, negative

75 DF formulation: Oral LD_{50} rat, 2416 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h Inhalation LC_{50} rat, >none; Primary eye irritation rabbit, mild; Skin irritation rabbit, slight; Skin sensitization guinea pig, negative

Chronic toxicity:

Rat and mouse chronic studies showed that sulfentrazone is not carcinogenic when administered to these animals in a lifetime study. There were adverse effects in multigeneration reproduction of rats, including effects on the growth and survival of the offspring, on the testes, and on sperm production.

Teratogenicity:

Rat oral teratology: Maternal NOEL, 25 mg/kg/d; fetal NOEL, 10 mg/kg/d

Rat dermal teratology: Maternal NOEL, >250 mg/kg/d; fetal NOEL, 100 mg/kg/d

Rabbit oral teratology: Maternal NOEL, 100 mg/kg/d; fetal NOEL, 100 mg/kg/d

Mutagenicity:

A number of mutagenicity studies have been conducted with sulfentrazone, including an Ames assay, mouse lymphoma, and in vivo mouse micronucleous assay. The weight of the evidence suggests that sulfentrazone is not mutagenic.

Wildlife:

Sulfentrazone is considered slightly toxic to fish and aquatic invertebrates in laboratory test systems and practically non-toxic to avian species.

Bobwhite quail 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >2250 mg/mL; 8-d dietary LC_{50}, >5620 mg/kg; Daphnia 48-h EC_{50}, 60.4 mg/L; Bluegill sunfish 96-h LC_{50}, 93.8 mg/L; Rainbow trout 96-h LC_{50}, >130 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Sulfentrazone was introduced in 1991 by the FMC Corporation. It was first field tested in 1991 and in 1995 through 1997 was tested under an Experimental Use Permit. Registration in soybeans is expected in 1998.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): FMC

Reference(s):

1. USEPA, Office of Prevention, Pesticides and Toxic Substances. 1997. Pesticide Fact Sheet.

sulfometuron-methyl

CAS #: 74222-97-2 $2^{(B)}$

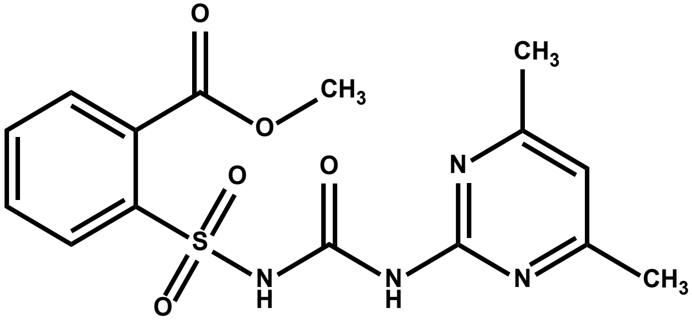
methyl 2-[[[[(4,6-dimethyl-2-pyrimidinyl)amino]carbonyl] amino]sulfonyl]benzoate

NOMENCLATURE

Common name: sulfometuron-methyl (ANSI, BSI, ISO, WSSA)
Other name(s): DPX-T5648; methyl 2-(4,6-dimethylpyrimidin-2-yl)carbamoylsulfamoyl)benzoate or methyl 2-[2-(4,6-dimethylpyrimidin-2-yl)ureidosulfonyl] benzoate (IUPAC)
Trade name(s): LANDMARK™ MP; LANDMARK™ II MP; LANDMARK™ XP; OUST® EXTRA; OUSTAR®; OUST®; SULFOMETURONMAX™; THROTTLE™ XP; WESTAR™; WESTAR™ HI
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
sulfometuron-methyl



Molecular formula: $C_{15}H_{16}N_4O_5S$
Molecular weight: 364.38 g/mole
Description: White solid, odorless
Density: 1.48 g/mL
Melting point: 203-205 C
Boiling point: NA
Vapor pressure: 7.2×10^{-14} Pa
Stability: NA
Solubility:
water, 10 mg/L (pH 5, 25 C); 300 mg/L (pH 7, 25 C)
organic solvents g/100 mL (25 C):
acetone 0.238
acetonitrile 0.153
ethanol 0.0137
ether 0.0032
xylene 0.0037
pK_a: 5.2 (weak acid) (3)
K_{ow}: NA

HERBICIDAL USE

Sulfometuron can be applied as follows: PRE or POST at 53-420 g ai/ha in conifer plantings or on sites to be transplanted to conifers; PRE or POST at 53-105 g ai/ha in dormant hardwood plantings or at 158-263 g ai/ha on sites to be transplanted to hardwoods; PRE or early POST at 70-420 g ai/ha or late fall/early winter at 53-210 g ai/ha in unimproved turf. Sulfometuron controls many annual and perennial broadleaf and grass weeds including annual sowthistle, common mallow, curly dock, western ragweed, barnyardgrass, foxtail barley, yellow foxtail, and jointed goatgrass. A nonionic surfactant improves sulfometuron efficacy, but may reduce selectivity when applying over-the-top in conifers.

USE PRECAUTIONS

Fire hazard: The product OUST® is dry and non-combustible.
Corrosiveness: The product OUST® is non-corrosive.
Storage stability: Stable
Cleaning glassware/spray equipment: Following an OUST® application, the spray tank should be used only for non-crop applications. Sulfometuron residues remaining in the tank may be dissolved in the next sprayer load and could be phytotoxic if applied POST to susceptible crops.
Emergency exposure: Flush eyes or skin with water; get medical attention if irritation persists.
Incompatibilities: Compatible with most commonly used non-cropland herbicides. Do not tank mix with high-pH herbicides.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth of treated plants is inhibited within a few h after application, but injury symptoms usually appear >2-3 wk later. Meristematic areas gradually become chlorotic, followed by general foliar chlorosis and necrosis. Plants may exhibit reddish-purplish coloration, vein discoloration, and necrosis of terminals.
Absorption/translocation: Readily absorbed into leaves following POST application and into roots from treated soil. Sulfometuron translocates in both xylem and phloem, although not extensively (1). Sulfometuron moves in the xylem and by mass flow with phloem solutes, accumulating in meristematic areas of the plant.
Metabolism in plants: Hydroxylation of the methyl carbon of the pyrimidine ring moiety followed by carbohydrate conjugation is the primary metabolic pathway for sulfometuron-methyl in wheat and bermudagrass (4).
Non-herbicidal biological properties: None known
.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: Average is 78 mL/g at pH 7 (3)
Transformation:
Photodegradation: Insignificant under field conditions
Other degradation: Microbial breakdown occurs slowly. Non-microbial hydrolysis is moderately rapid at pH 6, but extremely slow at pH 8. Thus, sulfometuron degradation occurs most rapidly at lower soil pH values where rates

are dominated by hydrolysis, whereas degradation rates are slowest at high pH and are dominated by microbial action. Non-microbial hydrolysis cleaves the sulfonylurea bridge.

Persistence: Typical field half-life is 20-28 d at pH 6-7 (3). Persistence is increased by cool temperatures, low soil moisture, and higher pH.

Mobility: Generally greater at higher soil pH and lower OM content

Volatilization: Insignificant losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade sulfometuron-methyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; inhalation 4-h LC_{50} rat, >5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

OUST: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} male rabbit, >8000 mg/kg, female rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL male 1000 mg/kg, clinical pathology effects at 5000 mg/kg

Chronic toxicity:

18-mo dietary, mouse: NOEL male 1000 mg/kg, female 1000 mg/kg; not oncogenic; mild anemia and body weight effects

24-mo dietary, rat: NOEL 50 mg/kg; not oncogenic

12-mo dietary, dog: NOEL 200 mg/kg anemia; hemolytic effect on erythrocytes at 1000 mg/kg

Teratogenicity:

Rat: NOEL 1000 mg/kg; not teratogenic; body weight effect at 5000 mg/kg

Rabbit: NOEL 300 mg/kg/d (highest level tested); not teratogenic

Reproduction:

Rat: NOEL 500 mg/kg in a 2-generation study; decreased body weight and pup counts at 5000 mg/kg; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative

Structural chromosome aberration: *In vitro* cytogenetics, negative

Wildlife:

Bobwhite quail 8-d dietary LD_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >5000 mg/kg, 8-d dietary LC_{50}, >5000 mg/kg; Daphnia 48-h LC_{50}, >12.5 mg/L; Bluegill sunfish 96-h LC_{50}, >12.5 mg/L; Rainbow trout 96-h LC_{50}, >12.5 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

NAMANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

sulfosulfuron

CAS #: 141776-32-1

2$^{(B)}$

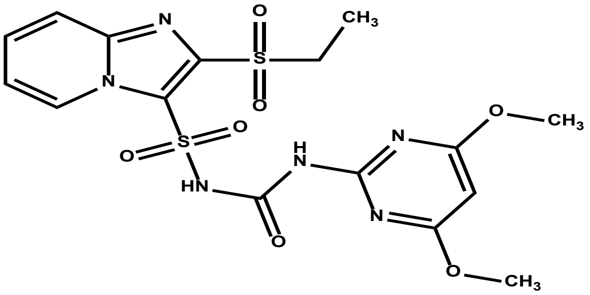
1-(4,6-dimethoxypyrimidin-2-yl)-3-[(2-ethanesulfonyl-imidazo[1,2-*a*]pyridine-3-yl]sulfonylurea

NOMENCLATURE

Common name: sulfosulfuron (ISO proposed)
Other name(s): MON 37500 (code number); TKM-19; 1-(4,6-dimethoxypyrimidin-2-yl)-3-(2-ethylsulfonylimidazo[1,2-*a*]pyridin-3ylsulfonyl)urea (IUPAC)
Trade name(s): APRYROS; CERTAINTY™; MAVERICK®; MAVERICK® PRO; MONITOR®; OUTRIDER®
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
sulfosulfuron



Molecular formula: $C_{16}H_{18}N_6O_7S_2$
Molecular weight: 470.47 g/mole
Description: White solid, odorless
Density: 1.52 g/mL (20 C)
Melting point: 201.1 – 201.7 C (technical)
Boiling point: NA
Vapor pressure: 8.81×10^{-8} Pa (25 C)
Stability: Stable
Solubility:
water (20 C):
17.6 mg/L (pH 5.0)
1627 mg/L (pH 7.0)
482 mg/L (pH 9.0)
pK$_a$: 3.51 (weak acid)
K$_{ow}$: <10 (pH 5.0 - 9.0)

HERBICIDAL USE

Sulfosulfuron can be applied PRE and POST to winter wheat, spring wheat, and triticale at 10-40 g ai/ha and POST in bermudagrass and bahiagrass roadsides at 26-70 g ai/ha. Weeds controlled include *Apera, Bromus* species, johnsongrass, *Phalaris* species, quackgrass, wild oats, and numerous broadleaf weeds including *Galium, Matricaria*, and mustard species.

USE PRECAUTIONS

Fire hazard: Technical and formulated products are dry and non-flammable.
Corrosiveness: Technical and formulated products are non-corrosive. and stable.
Cleaning glassware/spray equipment: Wash lab equipment with water and detergent, then rinse with acetone. Wash spray equipment with water and ammonia at 1% v/v and triple rinse with water.
Emergency exposure: Wash eyes with clean water for 15 min and get medical attention. Wash skin with soap and water.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS). (more details on page 12)
Symptomology: Rapid growth inhibition occurs with POST applications. Injury symptoms generally are observable within 7-14 days. Injury symptoms vary by species and generally include chlorosis and necrosis of the meristematic region followed by general foliar chlorosis and necrosis. Some species can remain in an inhibited growth pattern for an extended period after application, without showing injury symptoms.
Absorption/translocation: Foliar application of a pH 7.0 buffer solution of sulfosulfuron to wheat leaves results in absorption levels ranging from 40-65% after 7 days. Translocation in wheat is less than 10%. In downy brome, absorption levels ranged from 5-21% after 7 days, with translocation levels less than 5%.
Metabolism in plants: PRE application of sulfosulfuron to soil results in uptake of low levels of the herbicide, which comprised less than 10% of the plant residue. Numerous metabolites were observed, which constituted the remainder of the residues. The metabolite distribution in rotational crops (barley, radish, and lettuce) was different than in PRE-applied wheat, and resulted from almost exclusive uptake of soil metabolites. POST applications of sulfosulfuron to wheat gave residues consisting primarily of parent along with numerous low-level metabolites. Analysis of wheat extracts from a foliar application study showed that absorbed Sulfosulfuron was completely metabolized after 7 d at 25 C.
Non-herbicidal biological properties: None identified
Mechanism of resistance in weeds: Some weed biotypes have altered ALS binding sites causing certain ALS herbicides to be ineffective on those biotypes.

BEHAVIOR IN SOIL

Sorption: There appears to be no correlation between the percent organic matter in the soil and the adsorption of sulfosulfuron. Results, however, suggest that the adsorption of sulfosulfuron increases as pH decreases
K$_{oc}$: 5 to 89 mL/g using the Freundlich K.
Transformation:
Photodegradation: Extensive degradation was observed at pH 7.0 when sulfosulfuron was exposed to simulated sunlight. The half-life of sulfosulfuron was approximately 3 d.

Other degradation: Degraded by microbes and by non-microbial hydrolysis with rapid rates in low pH soils and moderate rates in higher pH soils. Under aerobic conditions, however, microbial degradation is slow and most degradation is by hydrolysis. Degradation is rapid in water-sediment systems in which the water is aerobic and an aerobic-anaerobic gradient exists.

Persistence: Somewhat persistent. Due to the high level of sulfosulfuron activity, very low level residues can persist in soil long enough to injure certain crops 1 to 3 yr after application, depending upon the soil and climate.

Field experiments: Half-lives in bare ground dissipation studies ranged from 14 to 75 d depending upon the climate and soil characteristics. The degradation rate can vary considerably with environmental conditions.

Lab experiments: Half-lives were as follows: 32 d in an aerobic silt loam with 0.8% OM and pH 7.5; 35 days in an aerobic sandy loam with 1.6% OM and pH 6.8; 147 d in an aerobic (aquatic) sandy loam sediment with 2.3% OM and pH 7.4.

Mobility: In field studies in North Dakota and Texas, no quantifiable residues of sulfosulfuron were found below 12 inches. In radiolabeled field studies in California and eastern Washington, sulfosulfuron was found mainly in the 0-6 inches layer.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade sulfosulfuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, 3.0 mg/L; Primary eye irritation rabbit, slightly irritating; Skin irritation rabbit, negative; Skin sensitization guinea pig, negative

Formulated product: NA

Subchronic toxicity:

90-d dietary, mouse: NOEL male 1144 mg/kg/d, female 887 mg/kg/d; equivocal decrease in alkaline phosphatase in females at 2123 mg/kg/d

90-d dietary, rat: NOEL 370 mg/kg/d; mild reductions in body weight and body weight gain in males and pregnant females at 20,000 mg/kg

90-d dietary, dog: NOEL male 300 mg/kg/d, female 100 mg/kg/d; urinary tract gross and microscopic effects resulting from calculi in urinary tissues, and increased BUN at 393 mg/kg/d or greater; small increase in bladder tumors in males with bladder stones at 943 mg/kg/d; no effects of any type in females

Chronic toxicity:

18-mo dietary, mouse: NOEL males 93 mg/kg/d, females 1388 mg/kg/d; in males, gross and microscopic effects resulting from calculi in urinary tissues, and increased BUN at 393 mg/kg/d or greater; small increase in bladder tumors in males with bladder stones at 943 mg/kg/d; no effects of any type in females

24-mo dietary, rat: NOEL males 24 mg/kg/d, females 30 mg/kg/d; decreased body weight gain in females at 20,000 mg/kg, urinary crystals/calculi and related urinary tract lesions in males at 5000 mg/kg and in females at 5000 mg/kg and greater; bladder tumors in two females at 5000 mg/kg were considered related to chronic bladder stone irritation; no treatment-related tumors in males

12-mo oral capsule, dog: NOEL 100 mg/kg/d; urinary tract gross and microscopic changes related to urinary crystals and/or stones at 500 mg/kg/d

Teratogenicity:

Rat: NOEL > 1000 mg/kg/d, no effects in any parameters at 1000 mg/kg/d

Rabbit: NOEL > 1000 mg/kg/d; no effects in any parameters at 1,000 mg/kg/d

Reproduction:

Rat: NOEL >1000 mg/kg/d; no effects in any parameters at 1000 mg/kg/d

Rabbit: NOEL > 1000 mg/kg/d; no effects in any parameters at 1000 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: Mouse micronucleus, negative; *in vitro* cytogenetics human lymphocytes), negative; *in vitro* cytogenetics (Chinese hamster lung cells), increases in chromosome aberrations were only observed in the absence of S9 mix at dose levels exceeding solubility (>2000 mg/mL) with precipitating test material present

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 5-d dietary LC_{50}, >5620 mg/kg, 1-generation reproduction NOEC 1250 mg/kg; Mallard duck oral LD_{50}, >2250 mg/kg, 5-d dietary LC_{50}, >5620 mg/kg, 1-generation reproduction NOEC 1250 mg/kg: Honey bee topical, >30 mg/bee; oral LD_{50}, >25 mg/bee; Daphnia, 48-h EC_{50}, >96 mg/L, 21-d Life cycle EC_{50}, >102 mg/L for immobilization and reproduction end points; Bluegill sunfish 96-h LC_{50}, >96 mg/L; Rainbow trout 96-h LC_{50}, >95 mg/L, Early Life Stage NOEC 100 mg/L for all parameters; Sheepshead minnow 96-h LC_{50}, >101 mg/L; Mirror carp 96-h LC_{50}, >91 mg/L; Mysid shrimp 96-h EC_{50}, 106 mg/L; Oyster 96-h shell deposition EC_{50}, 116 mg/L; *Selenastrum* (biomass) 72-h EC_{50}, 0.221 mg/L, 120-h EC_{50}, 0.367 mg/L, (growth) 72-h EC_{50}, 0.669 mg/L, 120-h EC_{50}, 0.954 mg/L; *Scenedesmus* 72-h EC_{50}, 3.1 mg/L; *Anabaena* 120-h EC_{50}, 0.77 mg/L; *Navicula* 120-h EC_{50}, >87 mg/L; *Skeletonema* 120-h, >103 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Synthesized and discovered by Takeda Chemical Industries, Ltd. of Japan.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Monsanto

tebuthiuron

CAS #: 34014-18-1 $7^{(C_2)}$

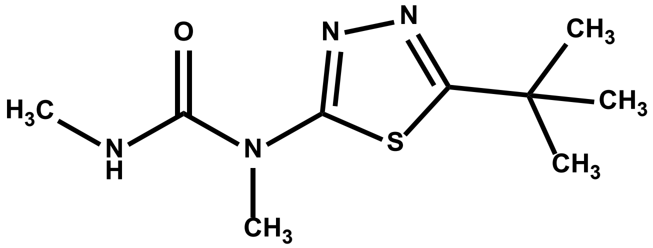
N-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-N,N'-dimethylurea

NOMENCLATURE

Common name: tebuthiuron (ANSI, BSI, ISO, WSSA)
Other name(s):; EL-103; 1-(5-*tert*-butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea (IUPAC)
Trade name(s): BRUSH-BULLET; COMBINE®; GRASLAN; SPIKE®; SPIKE® 20 P; SPIKE® 80 DF
Chemical family: substituted urea; thiadiazolylurea; urea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
tebuthiuron



Molecular formula: $C_9H_{16}N_4OS$
Molecular weight: 228.31 g/mole
Description: Colorless solid, slightly pungent odor
Density: 1.25 g/mL
Melting point: 161.5-164 C
Boiling point: Decomposes prior to boiling
Vapor pressure: 2.7 x 10^{-4} Pa (25 C)
Stability: Stable to UV light; decomposes near or above the melting point; stable in solutions of pH 5, 7, and 9 at 20 C, but hydrolyzes in strong alkali at high temperatures
Solubility:
water 2.57 g/L (20 C)
organic solvents g/100 mL (25 C):
acetone 7
acetonitrile 6
benzene 0.37
chloroform 25
n-hexane 0.61
methanol 17
methyl cellosolve 6
pK_a: None (non-ionizable)
K_{ow}: 67.1

HERBICIDAL USE

Tebuthiuron can be soil- or foliar-applied at 0.84-4.48 kg ai/ha in pasture and rangeland, and at 0.84-4.48 kg ai/ha in non-crop situations such as industrial sites. Tebuthiuron controls certain broadleaf weeds and woody brush species at low rates and controls most broadleaf, grass, and brush species at higher rates.

USE PRECAUTIONS

Fire hazard: All formulated products are dry and non-flammable.
Corrosiveness: Tebuthiuron technical and all formulated products are non-corrosive.
Storage stability: Stable to cold and heat
Cleaning glassware/spray equipment: Clean glassware and spray equipment with water.
Emergency exposure: Flush eyes and skin with water; get medical attention if irritation develops. If formulated products are ingested, drink 1-2 glasses of water and induce vomiting.
Incompatibilities: Compatible with most other herbicides

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: NA
Absorption/translocation: Readily absorbed into roots, less so into foliage (8); tebuthiuron is readily translocated following root absorption (5, 6)
Metabolism in plants: Primarily degraded by *N*-demethylation and hydroxylation of the terbutyl side chain (2)
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Strongly adsorbed to clay and to soils with high cation exchange capacity
K_{oc}: Average is 80 mL/g (9), but ranges from 22-91 mL/g
K_d: 0.11 mL/g for a sand with 0.5% OM and pH 7.7; 1.82 mL/g for a clay loam with 2.0% OM and pH 6.9
Transformation:
Photodegradation: Negligible losses
Other degradation: Degraded by microbes, primarily by *N*-demethylation. Rates of non-microbial hydrolysis are negligible
Persistence: Half-life is 12-15 mo in areas receiving 102-152 cm annual rainfall, but is considerably greater in low rainfall areas and in muck or other soils with high OM content.
Field experiments: See Johnson and Morton (4)
Mobility: In field studies, tebuthiuron and its degradation products seldom have been detected below the top 61 cm of soil. Little to no lateral movement has been observed after tebuthiuron has bound to clay and OM (1). Tebuthiuron surface mobility is limited due to its solubility and low K_d values, allowing it to move quickly into the soil.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity testing was conducted with technical grade tebuthiuron unless otherwise indicated.
Acute toxicity:
Oral LD50 rat, 644 1590 mg/kg, mouse, 579 mg/kg, rabbit, 286 mg/kg, cat, >200 mg/kg, dog, >500 mg/kg; Dermal LD50 rat, >5000 mg/kg, rabbit, >200 mg/kg; 4-h inhalation LC50, NA>5.78 mg/L; Skin irritation rabbit,

none to slight; Skin sensitization guinea pig and mouse, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, mouse: NOEL 83 mg/kg/d
90-d dietary, rat: NOEL 100 mg/kg/d
90-d dietary, dog: NOEL 12.5 mg/kg/d
28-d immunotoxicity, rat: not immunotoxic

Chronic toxicity:

18-mo dietary, mouse: NOEL NA; not carcinogenic at 200 mg/kg/d (highest dose tested)
24-mo dietary, rat: NOEL 50 mg/kg/d; no cumulative toxicity or serious effects at 80 mg/kg/d; not carcinogenic
12-mo dietary, dog: NOEL 25 mg/kg/d

Teratogenicity:

Rat: NOEL 80 mg/kg/d, NOAEL 180 mg/kg/d; not teratogenic; reversible reductions in weight gain
Rabbit: NOEL 25 mg/kg/d

Reproduction:

Rat: NOEL 20 mg/kg/d; no abnormalities and not a reproductive toxin at 56 mg/kg/d

Mutagenicity:

Gene mutation: Ames test, negative
Structural chromosome aberration: Mouse micronucleus, negative

Wildlife

Bobwhite quail oral LD_{50}, >2500 mg/kg; 8-d dietary LC_{50}, >5113 mg/kg; Mallard duck oral LD_{50} >2000 mg/kg; 8-d dietary LC_{50}, >5093 mg/kg; Chicken oral LD_{50}, >500 mg/kg; Earthworm 14-d LC_{50} in soil, 100 mg/kg; Honey bee 48-h contacy LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 297 mg/L; Bluegill sunfish 96-h LC_{50}, 106 mg/kg; Rainbow trout 96-h LC_{50},143 mg/L; green algae 96-h EC_{50}, 0.049 mg/L; duckweed 14-d EC_{50}, 0.235 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Pivalic acid and MTSC (4-methyl-3-thiosemicarbazide) are combined and a mix of sulfuric and polyphosphoric acids are added over time. Toward the end of this reaction, ammonium hydroxide is added to neutralize pH. The lower aqueous layer is removed and isopropylbenzene is added to form an intermediate amine. Then, 1,3-dimethylurea is added with HCl. All reactions are conducted under nitrogen. Finally, solvents are removed under vacuum and the resulting crystals are washed in water and dried.

Analytical methods: Product analysis by HPLC or by GLC with FID. Residues are determined by LC-MS, LC-UV, and GC-FPD.

Historical: Discovered in 1970 by Air Supply, Inc. and first reported in 1974 (7). It was introduced in Brazil in 1974 by Eli Lilly & Co. British patent 1,266,172. GRASLAN was first marketed in 1974.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

Reference(s):

1. Chang and Stritzke. 1977. Weed Sci. 25:184
2. Eaton, B. J. et al. 1976. Abstr. Weed Sci. Soc. Am. 199.3.
3. Hatzios, K. K. et al. 1980. Plant Physiol. 65:319.
4. Johnson and Morton. 1989. J. Environ. Qual. 18:433.
5. McNeil, W. K. 1982. PhD Dissertation, Oklahoma State Univ.
6. McNeil, W. K. et al. 1980. Proc. South. Weed Sci. Soc. 33:104.7. Schwer, J. F. 1974. Proc. 12th Br. Weed Control Conf. 2:847.
7. Steinert and Stritzke. 1977. Weed Sci. 25:390.
8. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

tembotrione

CAS #:: 335104-84-2

$27^{(F_2)}$

2-[2-chloro-4-(methylsulfonyl)-3-[(2,2,2-trifluoroethoxy) methyl]benzoyl]-1,3-cyclohexanedione

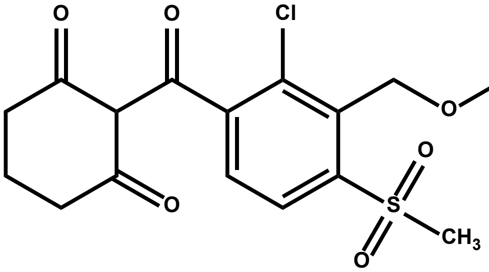
NOMENCLATURE

Common name: tembotrione (ISO approved in ?)
Other name(s): AE 0172747; 2-{2-chloro-4-mesyl-3-[(2,2,2-trifluoroethoxy)methyl]benzoyl}cyclohexane-1,3-dione (IUPAC),
Trade name(s): LAUDIS, SOBERAN, EQUINOX
Chemical family: Triketone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

tembotrione



Molecular formula: $C_{17}H_{16}ClF_3O_6S$
Molecular weight: 440.82 g/mole
Description: Beige powder
Density: 1.56 g ml^{-1}
Melting point: 123 C
Boiling point: decomposes before boiling
Vapor pressure: 1.1 x 10^{-05} mPa (25 C)
Stability:
Solubility:

Water: (20 C)

0.22 at pH 4
28.3 at pH 7
29.7 at pH 9

Organic solvents (g/L)

Ethanol	8.2
n-Hexane	47.6
Toluene	75.7
Ethyl Acetate	180.2

pH: 3.63
pK_a: 3.2
K_{ow}: log K_{ow} = 8.13 x 10^{-2}

HERBICIDAL USE

Registered for selective postemergence grass and broadleaf weed control in corn.

USE PRECAUTIONS

Fire hazard: not flammable
Corrosiveness: Non-corrossive
Storage stability: NA
Cleaning glassware/spray equipment: NA
Emergency exposure: .
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: 4-hydroxyphenylpyruvate dioxygenase inhibitor (more details on page 15)
Symptomology: General whitening of the apical meristem is observed a few days after application. This is followed by necrosis and death.
Absorption/translocation: Tembotrione is readily transported to meristems.
Metabolism in plants: In corn, 24 hours after application, 81.8 % of the extractable radioactive residue co-chromatographed with the metabolite 2-chloro-4-mesyl-3-[(2,2,2-trifluoroeth -oxy)methyl]benzoic acid 15.5 % with other metabolites, the rest with parent compound. (1)
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: Certain amaranthus species show an enhanced metabolism of tembtrione which renders them resistant to tembotrione.

BEHAVIOR IN SOIL

Sorption: K_f=1.59; K_{f0C}=66 (Adsorption increases as pH decreases) (2)
Transformation:
Photodegradation: Stable
Other degradation: .NA
Persistence: DT_{50} typical 14.5 days
Field experiments: DT_{50} 2.72 days
Mobility: GUS leaching potential index: 2.53 (calculated) (2)
Volatilization: Not volatile

TOXICOLOGICAL PROPERTIES

.Acute toxicity:

Oral LD_{50} rat, >2,500 mg/kg, Dermal LD_{50} rat, >2,000 mg/kg, Inhalation LC_{50} rat, >4.58 mg/l

Subchronic toxicity:

90-d dietary, rat: NOEL male 0.7 mg/kg,

Chronic toxicity: dog: LOAEL= M: 2.5 mg/kg/day; NOAEL=F: 10.2 mg/kg/day
Teratogenicity: Non-teratrogenic
Reproduction: Not a reproductive toxicant
Mutagenicity: Not a mutagen
Wildlife:

Birds oral LD_{50} >2,250 mg/kg, Fish Acute 96 hour LC_{50} >100, Honeybees Acute 48 hour LD_{50} >92.8 ug/bee

Use classification:

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

Reference(s):

1, Schulte, W. and H. Köcher 2009. Bayer CropScience Journal 62:35-52.
2. IUPAC chemical information: tembotrione http://sitem.herts.ac.uk/aeru/iupac/1118.htm

tepraloxydim

CAS #: 149979-41-9 **$1^{(A)}$**

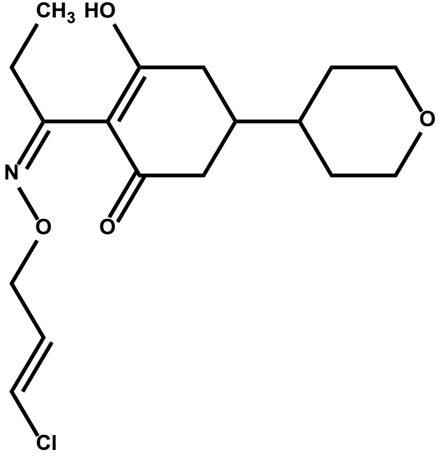
2-[1-[[[(2E)-3-chloro-2-propenyl]oxy]imino]propyl]-3-hydroxy-5-(tetrahydro-2H-pyran-4-yl)-2-cyclohexen-1-one

NOMENCLATURE

Common name: tepraloxydim (ISO)
Other name(s): (5RS)-2-{(EZ)-1-[(2E)-3-chlorallyloxyimino]propyl}-3-hydroxy-5-perhydropyran-4-ylcyclohex-2-en-1-one (IUPAC)
Trade name(s): EQUINOX®; FLAXMAX® DLX; ODYSSEY DLX
Chemical family: cyclohexanedione; cyclohexanedione oxime; cylcohexenone; cyclohexene oxime

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
tepraloxydim



Molecular formula: $C_{17}H_{24}ClNO_4$
Molecular weight: 341.83 g/mole
Description: Dark yellow clear liquid (product)
Density: 1.28 g/mL
Melting point: NA
Boiling point: NA
Vapor pressure: 2.7×10^{-5} Pa (25 C); Henry's Law constant, 8.74×10^{-9} kPa m^3/mole
Stability: Stable at 54 C for 14 d; reacted with iron acetate to form black liquid
Solubility: Water 430 mg/L (pH 6.5); 9.0 7250 mg/L (pH 9.0)

Solvent solubility (g/100 mL):

acetone	70
methanol	33
2-propanol	16
ethyl acetate	69
acetonitrile	77
dichloromethane	119
toluene	82
n-heptane	1
1-octanol	15
olive oil	8

pK_a: 4.58 (weak acid)
K_{ow}: log K_{ow} = 2.44 (pH 4); 0.20 (pH 7); -1.15 (pH 9); 1.5 (pure water) tepraloxydim is moderately persistent in flooded soils under anaerobic conditions.

HERBICIDAL USE

Tepraloxydim is used for the control of certain grass weeds in canola, chickpeas, faba beans, field peas, lentils, lupins, subcover and vetch.

USE PRECAUTIONS

Fire hazard: Although the material is not flammable, the concentrate is combustible. If involved in a fire, it will emit oxides of carbon, oxides of nitrogen and possibly hydrogen chloride or phosgene. Breathable air apparatus should be worn when fighting a fire in which this product is involved. Flash point is 93 C. Vapors may form explosive mixture with air. Prevent electrostatic charge – sources of ignition should be kept well clear – fire extinguishers should be kept handy.
Corrosiveness: NA
Storage stability: Hazardous polymerization is not possible; keep away from strong oxidizing agents. Protect from temperatures below -10 C or above 30 C. Changes in the properties of the product may occur if substance/product is stored above indicated temperature for extended periods of time. The product EQUINOX® is stable for 12 mo at 20 C, 50% relative humidity in polyamide-lined HDPE bottle.
Cleaning glassware/spray equipment: Thoroughly clean application equipment immediately after spraying. Ensure that all traces of the product are removed. Drain and flush tank walls, boom, and all hoses for 10 min with clean water. Do not clean the sprayer near desirable vegetation, wells, or other water sources. Remove the nozzles and screens and wash separately. Dispose of all rinsates in accordance with state and local regulations. If a broadleaf herbicide, insecticide, or fungicide tank mix partner is used, always check tank mix partner label for any additional cleanup procedures.
Emergency exposure: Causes moderate eye irritation. Avoid contact with eyes, skin or clothing; may be harmful to lungs if swallowed. If in eyes, hold eye open and rinse slowly an gently with water for 15-20 min. Remove contact lenses ,if present after the first 5 min, then continue rinsing eye. If on skin or clothing, take off contaminated clothing and launder before reuse. Rinse skin immediately with plenty of soap and water for 15-20 min. Call a poison control center or doctor for treatment advice. If swallowed, immediately call a poison control center or doctor. Do not induce vomiting unless told to do so by a poison control center or doctor as vomiting solvent may cause pulmonary pneumonitis. If inhaled, move person to fresh air until recovered. If symptoms develop or persist, seek medical advice. Call a poison control center or doctor for further treatment advice regarding exposure in eyes, skin, clothing, swallowing, or inhalation.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details on page 12)

Symptomology: Growth ceases within a few days of application with meristematic regions affected first. Leaf chlorosis and eventually necrosis develop within 1-3 wk of application. Leaf sheaths become brown and flaccid at and just above their point of attachment to the node. Older leaves often turn purple, orange, or red before becoming necrotic.

Absorption/translocation: Rapidly absorbed into roots and leaves; translocated predominately in the phloem

Metabolism in plants: NA

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: Similar to other ACCase-resistant weeds

BEHAVIOR IN SOIL

Sorption: K_d = 0.011 to 1.5 mL/g; K_{oc} = 3.7 to 77.2 mL/g

Transformation:

Photodegradation: Tepraloxydim has a potential for phototransformation in the environment, as the UV-visible spectra indicates an absorption maximum at 290-300 nm. Tepraloxydim phototransformed rapidly on a loamy sandy soil with a half-life of 1 d, which indicates that phototransformation is an important route of transformation in the soil environment.**Other degradation:** Hydrolysis of tepraloxydim is pH and temperature dependent. Tepraloxydim hydrolyzes slowly under neutral and alkaline conditions, but

Field experiments: Tepraloxydim dissipated rapidly with DT_{50} values of 6, 3, 12, and 9 d at the Manitoba, Saskatchewan, Alberta, and North Dakota sites, respectively. These values indicate that tepraloxydim is non-persistent under field conditions. No residues were detected below a depth of 5 cm at any site at any time; consequently, the parent compound and transformation products have a low potential to leach and contaminate groundwater under field conditions.

Mobility: Tepraloxydim is highly to very highly mobile in sand, sandy loam, loamy sand, loam and clay soils.

Volatilization: Non-volatile and no significant volatilization is expected.

hydrolyzes rapidly under acidic conditions (half-life 3.5 to 24.4 d). Hydrolysis is considered an important route of transformation of tepraloxydim under acidic conditions, whereas in neutral and alkaline conditions it may be a route of transformation at elevated temperatures.

Persistence:

Laboratory experiments: Tepraloxydim bio-transformed rapidly in a sandy laom soil under aerobic conditions with first-order half-lives of 5.3 and 9 d in cyclohexene ring-labelled and tetrahydropyran ring-labeled ^{14}C tepraloxydim studies, respectively. Half-life values indicate that tepraloxydim is non-persistent in the terrestrial environment under aerobic conditions. DT_{90} values ranged from 17 to 28 d. Under anaerobic conditions, tepraloxydim transformed in the flooded soil system with a first-order half-life and DT_{90} value of 3.2 mo and 10.5 mo, respectively. The first-order half-lives in water and soil were 3.2 and 3 mo, respectively. Half-life values indicate that tepraloxydim is moderately persistent in flooded soils under anaerobic conditions.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade tepraloxydim unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, > 2000 mg/kg; Dermal LD_{50} rat, > 2000 mg/kg; Inhalation (4-h) LC_{50} rat, 5.1 mg/L; Eye irritation rabbit, minimally irritating; Skin irritation, not irritating; Skin sensitizer, not a sensitizer

EQUINOX® herbicide: Oral LD_{50} rat, > 2000 mg/kg; Dermal LD_{50} rat, > 2000 mg/kg; Inhalation (4-h) LC_{50} rat, 5.4 mg/L; Eye irritation rabbit, moderately irritating; Skin irritation, moderately irritating; Skin sensitizer, not a sensitizer

Subchronic toxicity:

28-day dietary, mouse: NOAEL = 506 mg/kg/day (male), 664 mg/kg/day (female); LOAEL 1518 mg/kg/day (male), 2259 mg/kg/day (female)

28-day dietary, rat: NOAEL = 46 mg/kg/day (male), 49 mg/kg/day (female); LOAEL – 469 mg/kg/day, 89 mg/kg/day (female)

28-day dietary, dog: NOAEL not determined; LOAEL not determined

90-day dietary, mouse: NOAEL = 310 mg/kg/day (male), 424 mg/kg/day (female); LOAEL = 1484 mg/kg/day (female), 1912 mg/kg/day (female) based on clinical signs of toxicity fluid feces, vomit, pale and thin appearance, decreased activity, dehydration, cold to touch, and regurgitation in both sexes, and mucus in feces in the males) and decreased body weights, body weight gains, and food consumption in both sexes

90-day dietary, rat: NOAEL = 22 mg/kg/day (male), 26 mg/kg/day (female); LOAEL = 223 mg/kg/day (male), 257 mg/kg/day (female)

90-day dietary dog: NOAEL = 63.3 mg/kg/day (male), 68 mg/kg/day (female); LOAEL = 325 mg/kg/day (male), 358 mg/kg/day (female)

Chronic toxicity:

Dogs: NOAEL = 125 mg/kg/day; LOAEL was not observed

Mouse: NOAEL = 216.5 mg/kg/day (male) and 181.2 mg/kg/day (female)

Neurotoxicity:

Not neurotoxic

Teratogenicity:

NOAEL, Maternal = 120 mg/kg/day; developmental = 40 mg/kg/day; teratogenicity = 120 mg/kg/day; LOAEL, Maternal = 360 mg/kg/day; developmental = 120 mg/kg/day; teratogenicity = 360 mg/kg/day

Reproduction:

Rat: Parental NOAEL = 50.9 mg/kg/day (male), 54.7 mg/kg/day (female); Parental LOAEL = 253 mg/kg/day (male), 273.8 mg/kg/day (female); Reproductive NOAEL 253.1 mg/kg/day (male), 273.8 mg/kg/day (female)

Mutagenicity: Not mutagenic; not clastogenic

Wildlife:

Rainbow trout 96-h LC_{50}, >100 mg/L; bluegill sunfish 96-h LC_{50}, 78.2 mg/L; Daphnia magna 48- h EC_{50}, 7.44 mg/L; quail LD_{50} , > 2000 mg/kg; bees LD_{50}, > 200 µg/bee

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Reversed phase high-performance liquid chromatography/ultraviolet (HPCD/UV) method was provided for the determination of the active ingredient, tepraloxydim, in the technical product. Based on the validation data and the chromatograms provided, the method was assessed to be sufficiently specific, precise and accurate.

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): BASF; Nufarm

Reference(s):

1. Alternative Strategies and Regulatory Affairs Division, Pest Management Regulatory Agency. 2004. Proposed Regulatory Decision Document PRDD2004-01: Tepraloxydim, Equinox EC, Dash HC
.2. BASF. 2006. Material Safety Data Sheet: Equinox EC Herbicide. Revision date: 2005/11/04, (30326684/MDS_GEN_CA/EN)

terbacil

CAS #: 5902-51-2 **$5^{(C_1)}$**

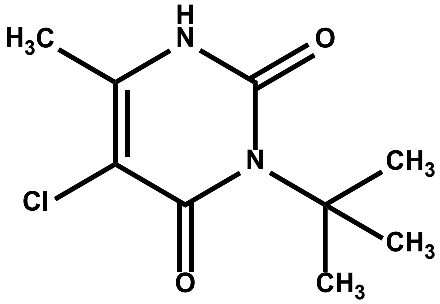
5-chloro-3-(1,1-dimethylethyl)-6-methyl-2,4-(1*H*,3*H*)-pyrimidinedione

NOMENCLATURE

Common name: terbacil (ANSI, BSI, ISO, WSSA)
Other name(s): DUPONT HERBICIDE 732; 3-*tert*-butyl-5-chloro-6-methyluracil (IUPAC)
Trade name(s): SINBAR®
Chemical family: uracil; substituted uracil

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
terbacil



Molecular formula: $C_9H_{13}ClN_2O_2$
Molecular weight: 216.67 g/mole
Description: White crystalline solid, odorless
Density: 1.34 g/mL (25 C)
Melting point: 175-177 C
Boiling point: NA
Vapor pressure: 4.1×10^{-8} Pa (25 C); 6.3×10^{-5} Pa (29.5 C); 7.2×10^{-4} Pa (54 C)
Stability: Stable to hydrolysis in water
Solubility:
- water 710 mg/L (25 C)
- organic solvents g/100 mL (25 C):
- butyl acetate 8.8
- methylisobutylketone 12.1
- cyclohexanone 18 xylene 6.1
- dimethylformamide 25.2

pK_a: 9 (weak base) (8)
K_{ow}: 78

HERBICIDAL USE

Terbacil can be applied as follows: POST at 0.45-1.34 kg ai/ha on dormant established alfalfa; PRE at 0.9-1.79 kg ai/ha or POST at 0.9-1.34 kg ai/ha in mint; soil-applied before weed emergence at 1.79-2.69 kg ai/ha in pecans; soil-applied before weed emergence at 0.9-1.79 kg ai/ha in small fruits; PRE at 0.9-2.24 kg ai/ha in sugarcane; and soil-applied (before weed emergence) at 1.79-3.58 kg ai/ha in deciduous tree fruits. Terbacil controls many annual broadleaf and grass weeds including common chickweed, henbit, lambsquarters, tansymustard, prickly lettuce, crabgrass spp., downy brome, foxtail spp., ryegrass, and barnyardgrass, with partial control of nutsedge.

USE PRECAUTIONS

Fire hazard: The product SINBAR is dry and non-flammable.
Corrosiveness: The product SINBAR is non-corrosive.
Storage stability: Terbacil technical is chemically stable under normal storage conditions.
Cleaning glassware/spray equipment: Flush equipment with water after removing nozzle tips and screens (clean these parts separately). Clean glassware by washing with detergent followed by acetone rinse.
Emergency exposure: May irritate eyes, nose, throat, and skin
Incompatibilities: The product SINBAR 80W is compatible with most herbicides with which it might be mixed.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Foliar chlorosis and inhibition of root and shoot growth
Absorption/translocation: Readily absorbed by roots, but less so by foliage and stems. Root-absorbed terbacil is translocated acropetally into leaves (4)
Metabolism in plants: Terbacil is metabolized in several species by oxidation and subsequent glucoside conjugation to the major metabolite, 3-*tert*-butyl-5-chloro-6-hydroxymethyl uracil (6).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Terbacil resistance was detected in Powell amaranth (2). Photosystem II activity of isolated thylakoids from the resistant biotype was 55-fold more resistant to terbacil than that of the susceptible biotype. Isolated thylakoids had lower binding affinity for terbacil than did thylakoids from susceptible biotypes (1).

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil colloids; the amount of terbacil adsorbed on Keyport silt loam soil in equilibrium with 1 mg/kg in soil solution was 1.7 mg/kg compared with 1.5 mg/kg of bromacil, 2.6 mg/kg of monuron, and 4.0 mg/kg of diuron (7).
K_{oc}: Average is 55 mL/g (8)
Transformation:
Photodegradation: Slowly photodegrades in water
Other degradation: Degraded microbially
Persistence: Somewhat long residual with an average field half-life of 120 d (8)
Field experiments: Half-life was ~5-6 mo when 4.5 kg ai/ha was applied to a Butlertown silt loam (4)
Mobility: Helling mobility class 3 (5)
Volatilization: Insignificant losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade terbacil unless otherwise indicated.

Acute toxicity:

Oral LD_{50} male rat, 1255 mg/kg; female rat, 934 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >4.4 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

Subchronic toxicity:

90-d dietary, rat: NOEL male 500 mg/kg

Chronic toxicity:

24-mo dietary, mouse: NOEL 50 mg/kg; not oncogenic

24-mo dietary, rat: NOEL 50 mg/kg; not oncogenic; liver effects

24-mo dietary, dog: NOEL 250 mg/kg

Teratogenicity:

Rat: NOEL 250 mg/kg; not teratogenic; fetotoxicity at 1250 and 5000 mg/kg/d

Rabbit: NOEL 200 mg/kg/d; not teratogenic; fetotoxicity at 600 mg/kg/d

Reproduction:

Rat: NOEL 250 mg/kg (highest level tested) in a 2-generation study

Mutagenicity:

Gene mutation: CHO, negative

Structural chromosome aberration: *In vivo* cytogenetics, negative

DNA damage/repair: *In vivo* UDS, negative

Wildlife:

Peking duckling 8-d dietary LC_{50}, >56,000 mg/kg; Pheasant chick 8-d dietary LC_{50}, >31,450 mg/kg; Honey bee, nontoxic; Pumpkinseed sunfish 24-h and 48-h TL_m, 86 mg/L; Fiddler crab 48-h LC_{50}, >1000 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Recrystallize twice from absolute ethanol

Analytical methods: Residues of terbacil and three metabolites in plant and animal tissue and in soil are determined by extraction with chloroform, cleanup by liquid/liquid partitioning, and measurement by halogen-sensitive microcoulometric GC after formulation of silyl derivatives of the metabolites. Method sensitivity is 40 ∝g/kg for all compounds relative to a 25-g sample.

Historical: Substituted uracils were first described as herbicides in 1962 (3). Introduced by Du Pont Company; U.S. patent 3,235,357 and Belgian patent 625,897.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

Reference(s):

1. Boydston and Al-Khatib. 1991. Proc. West. Soc. Weed Sci. 44:21.
2. Boydston and Al-Khatib. 1992. Weed Sci. 40:513.
3. Bucha, H. C. et al. 1962. Science 137:537.
4. Gardiner, J. A. et al. 1969. J. Agric. Food Chem. 17:980.
5. Helling and Turner. 1968. Science 162:562.
6. Lamoureux, G. L. et al. 1991. Pages 227-261 *in* J. C. Caseley, G. W. Cussans, and R. K. Atkin, eds., Herbicide Resistance in Weeds and Crops. Butterworth-Heinemann, Ltd., Oxford.
7. Rhodes, R. C. et al. 1970. J. Agric. Food Chem. 18:524.
8. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

terbumeton

CAS #: 33693-04-8 $5^{(C_1)}$

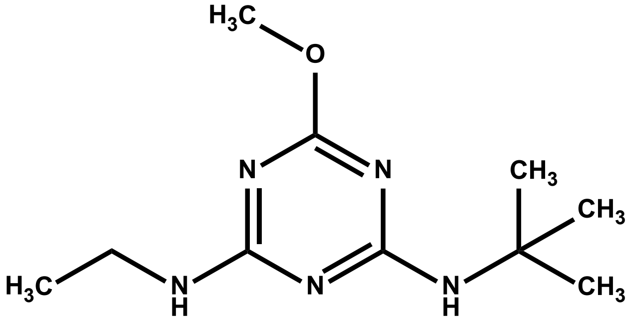
N-(1,1-dimethylethyl)-*N′*-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: terbumeton (ISO)
Other name(s): GS 14 259; N^2-*tert*-butyl-N^4-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine (IUPAC)
Trade name(s): CARAGARD®
Chemical family: methoxy-*s*-triazine; methoxy triazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
terbumeton



Molecular formula: $C_{10}H_{19}N_5O$
Molecular weight: 225.29 g/mole
Description: Colorless crystals
Density: 1.08 g/mL
Melting point: 123-124 C
Boiling point: NA
Vapor pressure: 2.7 x 10^{-4} Pa (20 C)
Stability: Stable in neutral, weakly acidic, and weakly alkaline media; hydrolyzed by strong acids and alkalis.
Solubility: In water, 130 mg/L (20 C), acetone 130 mg/L, methanol 220 mg/L, dichloromethane 360 mg/L
pK_a: 4.6 (21 C) (weak base)
K_{ow}: 1097

HERBICIDAL USE

Terbumeton is used for selective control of annual and perennial grasses and broadleaf weeds in citrus orchards. It is used in combination with terbuthylazine for weed control in vineyards, apple and citrus orchards, and in forestry at 3 to 6 kg a.i./ha. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA
Corrosiveness: Non-corrosive
Storage stability: NA
Emergency exposure: If ingested, induce vomiting and seek medical attention.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)
Symptomology: Chlorosis followed by necrosis of affected plant tissue
Absorption/translocation: Absorbed by roots and leaves; predominately xylem translocated
Metabolism in plants: NA
Mechanism of resistance in weeds: Altered target site

BEHAVIOR IN SOIL

Sorption:
K_d: 0.6-8.9 mL/g
K_{oc}: 37.5-158 mL/g
Transformation:
Other degradation: Undergoes microbial demethylation to the hydroxytriazine metabolite
Persistence:
Field experiments: DT_{50} = 300 d
Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.
Acute toxicity:
Oral LD_{50} rat, 483-657 mg/kg; Dermal LD_{50} rat, 3170 mg/kg; non-irritating to skin; slightly irritating to eyes
Subchronic toxicity:
90-d dietary, rat: NOEL 150 mg/kg/d
90-d dietary, dog: NOEL 25 mg/kg/d
Wildlife:
LC_{50} (96 h) for rainbow trout, 14 mg/L; channel catfish 10 mg/L; bluegill sunfish 30 mg/L; crucian carp; 30 mg/L; non-toxic to bees; LC_{50} Daphnia (48 h), 40 mg/L
Use classification: WHO class II; EPA (formulation) II

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

terbuthylazine

CAS #: 5915-41-3 **5$^{(C1)}$**

6-chloro-*N*-(1,1-dimethylethyl)-*N′*-ethyl-1,3,5-triazine-2,4-diamine

NOMENCLATURE

Common name: terbuthylazine (ISO)

Other name(s): TE-020; GS-13529; N^2-*tert*-butyl-6-chloro-N^4-ethyl-1,3,5-triazine-2,4-diamine (IUPAC)

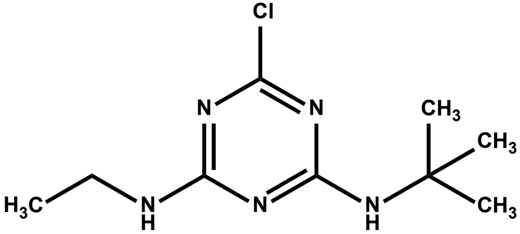
Trade name(s): AGPRO TERBUTHYLAZINE 500; CUNA®; GARDOTOP®; GARDOPRIM; MASCOT®; TOPOGARD 50

Chemical family: chloro-*s*-triazine; chlorotriazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

terbuthylazine



Molecular formula: $C_9H_{16}ClN_5$

Molecular weight: 229.71 g/mole

Description: colorless crystals

Density: 1.19 g/mole

Melting point: 177-179 C

Boiling point: NA

Vapor pressure: 1.5×10^{-4} Pa (20 C)

Stability: Stable in neutral, weakly acidic, and weakly alkaline media; hydrolyzed by strong acids and alkalis solution

Solubility: In water, 8.5 mg/L (20 C). In ethyl acetate 40 g/L; isopropanol 10 g/L; xylem 10 g/L

pK_a: 2.0 (weak base)

K_{ow}: $\log K_{ow} = 3.04$ (non-ionized form)

HERBICIDAL USE

Terbuthylazine is used for broad-spectrum pre-emergence and post-emergence weed control in maize, sorghum, vines, fruit trees, citrus, coffee, oil paom, cocoa, olives, potatoes, pease, beans, sugarcane, rubber, and in forestry in tree nurseries and new plantings. It is applied at 0.5 to 3 kg a.i./ha. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: Non-corrosive

Storage stability: NA

Emergency exposure: NA

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)

Symptomology: Chlorosis followed by necrosis of affected plant tissue

Absorption/translocation: Absorbed by roots and translocated predominately in the xylem; accumulates in apical meristem

Metabolism in plants: In tolerant plants, terbuthylazine is metabolized to hydroxyl triazine

Mechanism of resistance in weeds: Altered target site

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 162-278 mL/g

Transformation:

Photodegradation: In sunlight, DT_{50} <40 d

Other degradation: Microbial degradation to form the deethylterbuthylazine metabolite; hydrolysis DT_{50} is 8 d (pH 1), 86 d (pH 5), and >200 d (pH 9) and 12 d (pH 13)

Persistence:

Field experiments: DT_{50} 88-116 d

Volatilization: Non-volatile

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade terbuthylazine unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 2160 mg/kg; Dermal LD_{50} rat, 3000 mg/kg; Acute inhalation LC_{50} (4 h), >3.5 mg/L; slight skin irritant and non-irritant to eye (rabbit)

Subchronic toxicity:

90-d dietary, rat: NOEL 3.5 mg/kg/d

Wildlife:

Acute oral LD_{50} for duck and quail, >1000 mg/kg; Dietary LC_{50} (8 d) for duck and quail, > 65620 mg/kg; LC_{50} (96 h) for rainbow trout, 3.8-4.6; bluegill sunfish, 7.5; carp and catfish, 7.0 mg/L; Bee LD_{50} (oral and contact), >100 µg/bee. No effects on bacterial respiration and nitrification in range 10.9-109 mg/kg soil

Use classification: WHO class V; EPA (formulation) 3

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Roberts, T. R. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.

thenylchlor

CAS #: 96491-05-3

$15^{(K_3)}$

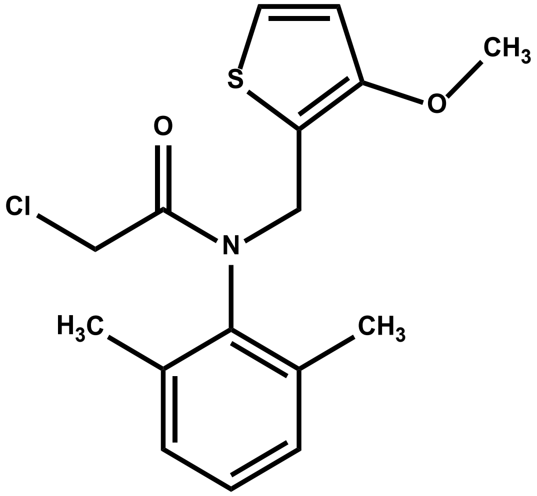
2-chloro-*N*-(2,6-dimethylphenyl)-*N*-[(3-methoxy-2-thienyl) methyl]acetamide

NOMENCLATURE

Common name: thenylchlor
Other name(s): NSK-850; 2-chloro-*N*-(3-methoxy-2-thenyl)-2',6'-dimethylacetanilide (IUPAC)
Trade name(s): ALHERB; KINGDOM FLOWABLE; ONE BEST FLOWABLES; PAPIKA A1 KILO; PRECUT; STEP FLOWABLE
Chemical family: acetamide; acetanilide; chloroacetamide; chloroacetanilide

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
thenylchlor



Molecular formula: $C_{16}H_{18}ClNO_2S$
Molecular weight: 323.84 g/mole
Description: White solid with slight sulfurous odor
Density: 1.19 g/mL (25 C)
Melting point: 72-74 C
Boiling point: 173-175 C (6.66 Pa)
Vapor pressure: 2.8×10^{-5} Pa (25 C)
Stability: Decomposes at 260 C; decomposed by ultraviolet radiation (400 nm, 8 h); stable to acid and base in range of pH 3-8
Solubility: In water, 11 mg/L (20 C)
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 3.53 (pH 7, 25 C)

HERBICIDAL USE

Thenylchlor is used for preemergence control of annual grasses (particularly *Echinochloa crus-galli*) in paddy rice at 300 – 500 g a.i./ha; not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: Flammable at 224 C
Corrosiveness: NA
Storage stability: NA
Emergency exposure: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of shoot growth; recent data indicates chloroacetamides inhibit very long chain fatty acid synthesis (more details on page 14)
Symptomology: Inhibition of seedling shoot growth.
Absorption/translocation: Absorbed through roots; predominately xylem translocated.
Metabolism in plants: In rice, thenylchlor is metabolized to water-soluble products.
Mechanism of resistance in weeds: No reported resistance

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 480-2846 mL/g**Transformation:**
  Other degradation: Microbial degradation yields dechlorinated thenylchlor, *N*-dealkylated product, aryl hyrdoxyaltion, and *O*-demethylated thenylchlor.
Persistence:
  Lab experiments: DT_{50} 1-3 weeks
Volatilization: Moderate

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade thenylchlor unless otherwise indicated.

Acute toxicity:
  Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4 h inhalation LC_{50} rats, >5.67 mg/L
  Chronic toxicity:Rat: NOEL 6.84 mg/kg/d
Wildlife:
  Bobwhite quail acute LD_{50}, > 2000 mg/kg; 96 h bees LD_{50}, >100 µg/bee; earthworm 14 d LD_{50}, >1000 mg/kg
Use classification: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Tokuyama
Reference(s):

1. Roberts, T. 1998. Metabolic Pathways of Agrochemicals. Royal Society of Chemistry.

thiazopyr

CAS #: 117718-60-2 $3^{(K_1)}$

methyl-2-(difluoromethyl)-5-(4,5-dihydro-2-thiazoly)-4-(2-methylpropyl)-6-(trifluoromethyl)-3-pyridinecarboxylate

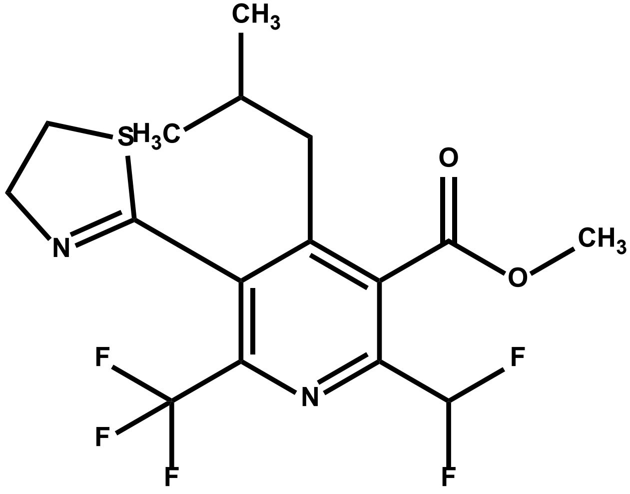
NOMENCLATURE

Common name: thiazopyr (ANSI, ISO,WSSA)
Other name(s): MON 13200; RH-123652; methyl 2-difluoromethyl-5-(4,5-dihydro-1,3-thiazol-2-yl)-4-isobutyl-6-trifluoromethylnicotinate (IUPAC)
Trade name(s): MANDATE™; SPINDLE; VISOR™
Chemical family: pyridine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

thiazopyr



Molecular formula: $C_{16}H_{17}F_5N_2O_2S$
Molecular weight: 396.38 g/mole
Description: Light tan crystalline solid, slight sulfur odor
Density: 1.37 g/mL (25 C)
Melting point: 77.3-79.1 C
Boiling point: 236-282 C
Vapor pressure: 2.67 x 10^{-4} Pa (25 C)
Stability: NA
Solubility:
water 2.5 mg/L (20 C)
organic solvents g/100 mL (20 C):
n-hexane 3.1
methanol 28.7
pK_a: None (non-ionizable)
K_{ow}: 7729 (21 C)

HERBICIDAL USE

Thiazopyr can be soil-applied at 0.1-2.24 kg ai/ha for control of grasses and certain small-seeded broadleaf weeds. It has selectivity in several crops including alfalfa, cotton, peanuts, soybeans, tree crops, and vines. Limited testing has indicated its potential for use in sunflowers, sugarcane, transplanted vegetables, potatoes, small fruits and berries, and in forestry and industrial sites.

USE PRECAUTIONS

Fire hazard: EC formulation is non-flammable; flash point is (>93 C).
Corrosiveness: NA
Storage stability: Shelf-life of dry formulations is expected to be >2 yr under storage at <35 C.
Cleaning glassware/spray equipment: NA
Emergency exposure: Wash skin with soap and water.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Disrupts cell division by inhibiting mitosis in late prometaphase (more details on page 12)
Symptomology: Root growth inhibition and swelling in meristematic regions such as root tips. Susceptible plants may show thickened or swollen hypocotyls or intermodes. Seed germination is not inhibited.
Absorption/translocation: NA
Metabolism in plants: Thiazopyr is extensively and rapidly degraded to a large number of polar metabolites, each comprising <10% of the total applied thiazopyr residues. Major degradation reactions include sulfur oxidation, thiazoline ring opening and methyl ester hydrolysis, and transformation of the isobutyl side chain. The 2-difluoromethyl-4-(2-methylpropyl)-6-trifluoromethyl-3-(pyridinecarboxylate moiety is found in most of the metabolites as well as in the parent thiazopyr.
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: NA

BEHAVIOR IN SOIL

Sorption: NA
Transformation:
Photodegradation*:* Thiazopyr degraded with half-loves of 7.8 and 20.8 d, respectively, in unsensitized and humic acid sensitized sterile aqueous pH 5 buffer solutions using artificial sunlight at 25 C. Photodegradation on soil in insignificant.
Other degradation: Thiazopyr is stable in sterile aqueous buffered solutions at pH 4 and 5. Hydrolysis was observed at pH 7 and 9, with predicted half-lives of thiazopyr of 3394 d and 64 d, respectively. Degraded primarily by microbes and secondarily by non-microbial hydrolysis. Half-lives were 111 and 437 d in loam soil and in a sandy soil, respectively. The monoacid degradation product was produced at low levels 20 d after application.
Persistence: Half-life averages 64 d, but ranged from 8-437 d. Dissipation rate varies with temperature, moisture, soil, pH, and organic matter content. Wheat, grain sorghum, and sugarbeets are especially susceptible to soil residues of thiazopyr and may require rotational intervals.
Mobility: Low mobility; thiazopyr has seldom been detected below 46 cm across numerous soils and agricultural regions in the U.S.
Volatilization: Insignificant losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade thiazopyr unless otherwise indicated.

Acute toxicity:

Oral LD$_{50}$ rat, >5000 mg/kg; Dermal LD$_{50}$ rabbit, >5000 mg/kg; 4-h inhalation LC$_{50}$ rat, >1.2 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity: NA

Chronic toxicity: NA

Teratogenicity:

Rat and rabbit: NOEL NA; not teratogenic

Reproduction:

Rat: NOEL NA; not a reproductive toxin

Mutagenicity: No evidence of mutagenicity or genotoxicity in several tests

Wildlife:

Bobwhite quail oral LD$_{50}$, 1913 mg/kg, 8-d dietary LC$_{50}$, >5620 mg/kg; Mallard duck 5-d dietary LC$_{50}$, >5620 mg/kg; Honey bee oral LC$_{50}$, >1000 mg/kg, topical LD$_{50}$, >100 ∝g/bee; Daphnia 48-h LC$_{50}$, 5.9 mg/L; Bluegill sunfish 96-h LC$_{50}$, 3.4 mg/L; Rainbow trout 96-h LC$_{50}$, 3.2 mg/L

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Gas chromatography with mass spectrometry. Limit of quantitation is 0.025 mg/kg.

Historical: U.S. patent 4,988,384 was issued to Monsanto.

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): None

Reference(s):

1. Ambruster, B.L. et al. 1991. Pestic. Biochem. Physiol. 40:48.
2. Vaughn and Lehnen. 1991. Weed Sci. 39:450.
3. USEPA. 1997. Thiazopyr Pesticide Fact Sheet. Office of Prevention, Pesticides and Toxic Substances. 13 pp.

thiencarbazone-methyl

CAS #::317815-83-1 $2^{(B)}$

methyl 4-[[[(4,5-dihydro-3-methoxy-4-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl)carbonyl]amino]sulfonyl]-5-methyl-3-thiophenecarboxylate

NOMENCLATURE

Common name: Thiencarbazone-methyl ISO

Other name(s): methyl 4-[(4,5-dihydro-3-methoxy-4-methyl-5-oxo-1*H*-1,2,4-triazol-1-yl) carbonylsulfamoyl]-5-methylthiophene-3-carboxylate (IUPAC)

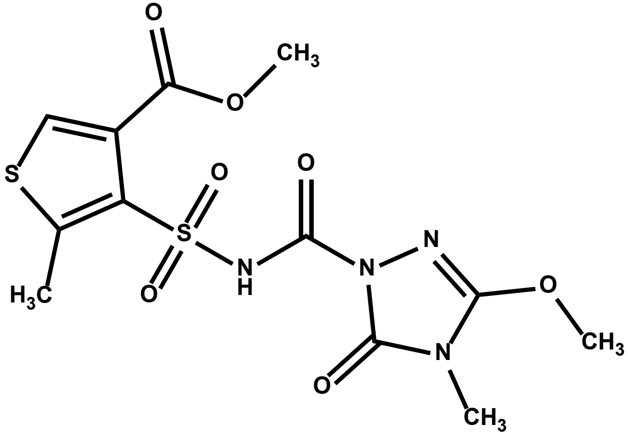
Trade name(s): CORVUS, ADENGO, CAPRENO

Chemical family: sulfonylaminocarbonyltriazolinone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

thiencarbazone-methyl



Molecular formula: $C_{12}H_{14}N_4O_7S_2$

Molecular weight: 390.44 g/mole

Description: white crystalline powder

Density: 1.51 g ml^{-1}

Melting point: 206 °C

Boiling point: decomposes before boiling

Vapor pressure: ~9 x 10-14 Pa (20 ºC, extrapolated)

Stability:

Solubility:

Water:
172 mg/L at pH 4
436 mg/L at pH 7
417 mg/L at pH 9
Organic solvents at g/L 20 °C

Ethanol	0.23
n-Hexane	0.00015
Toluene	0.19
Dichloromethane	100-120
Acetone	9.54
Ethyl acetate	2.19
Dimethyl sulfoxide	29.15

pK_a: 3.0

K_{ow}: log K_{ow} = -0.13 at pH 4, 24 °C;
-1.98 at pH 7, 24 °C;
-2.14 at pH 9, 23 °C

HERBICIDAL USE

Thiencarbazone-methyl is registered for selected grass and broadleaf control in corn premergence and postemergence in combination with isoaxflutole and tembotrione.

USE PRECAUTIONS

Fire hazard: nonflammable

Corrosiveness: NA

Storage stability: NA

Cleaning glassware/spray equipment: NA

Emergency exposure: .NA

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Growth of treated plants is inhibited within hr after application, but injury symptoms usually appear >1-2 wk later. Meristematic areas gradually become chlorotic and necrotic, followed by a general foliar chlorosis and necrosis.

Absorption/translocation: Rapidly absorbed by foliage and roots and translocates extensively in xylem and phloem after foliar applications with accumulation in meristematic areas.

Metabolism in plants:

Non-herbicidal biological properties: NA

Mechanism of resistance in weeds: Sulfonylurea-resistant weed biotypes selected in the field by chlorsulfuron use typically are resistant to tribenuron-methyl. The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: NA

Transformation:

Photodegradation: NA

Other degradation: .NA

Persistence: DT_{50} 11.6 days (typical)

Field experiments: DT_{50} 17 days

Mobility: NA

Volatilization: non-volatile

TOXICOLOGICAL PROPERTIES

.Acute toxicity:

Acute Oral – rat LD_{50}>2,000 mg/kg
Acute Dermal – rat LD_{50}>2,000 mg/kg
Acute Inhalation – rat LC_{50}>2.018 mg/L

Subchronic toxicity: 90 day dietary rat**:** NOAEL = 123 in males and 154 mg/kg/day in females.

Chronic toxicity: Rat: NOAEL = 234 for males and 313.4 for females mg/kg/day (1)

Teratogenicity: NA

Reproduction: There is no indication of increased susceptibility of rat or rabbit offspring to thiencarbazone-methyl as indicated by the rat and rabbit developmental toxicity studies and the rat reproduction study. There is no concern for increased susceptibility to offspring.

Mutagenicity: None of the battery of mutagenicity or genetic toxicity studies for thiencarbazone-methyl indicated a positive result.

Wildlife:

Acute

Birds LD_{50} >2,000 mg/kg
Fish 96 hour LC_{50} (mg l-1) > 104
Aquatic invertebrates 48 hour EC_{50}
(mg l-1)> 98.6
Honeybees - 48 hour LD_{50}
(μg bee-1) > 199

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: NA
Historical: **NA**

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience
Reference(s):

1, EPA Pesticide Fact Sheet: Thiencarbazone-methyl 2008. http://www.epa.gov/opp00001/chem_search/reg_actions/registration/fs_PC-015804_30-Oct-08.pdf
2.

thifensulfuron-methyl

CAS #: 79277-27-3 **$2^{(B)}$**

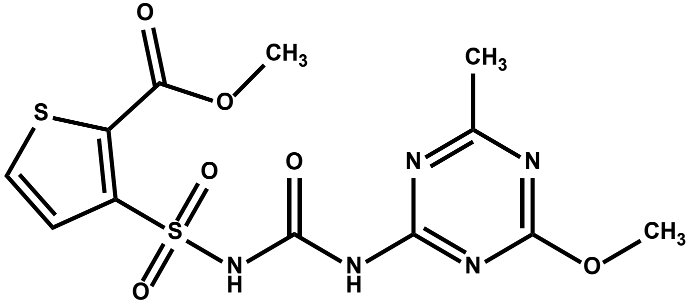
methyl 3-[[[[(4-methoxy-6-methyl-1,3-5-triazin-2-yl)amino] carbonyl]amino] sulfonyl]-2-thiophenecarboxylate

NOMENCLATURE

Common name: thifensulfuron-methyl (ANSI, ISO, WSSA)
Other name(s): DPX-M6316; thiameturon-methyl (discontinued common name); methyl 3-(4-methoxy-6-methyl-1,3,5-triazin-2-ylcarbamoylsulfamoyl) thiophene-2-carboxylate (IUPAC)
Trade name(s): AFFINITY™; AFFINITY™ BROADSPEC; AFFINITY™ TANKMIX; ALLY® EXTRA; BASIS ®; CANVAS®; CHEYENNE®; HARMONY®; HARMONY®EXTRA HARMONY® GT XP; HARMONY® EXTRA XP; PINNACLE®; STOUT; STOUT (MP); SUPREMACY®; SYNCHRONY®; SYNCHRONY® STS; SYNCHRONY® XP
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:*thifensulfuron-methyl*



Molecular formula: $C_{12}H_{13}N_5O_6S_2$
Molecular weight: 387.39 g/mole
Description: White solid, odorless
Density: 1.49 g/mL
Melting point: 186 C
Boiling point: NA
Vapor pressure: 1.7×10^{-8} Pa (25 C); Henry's Law constant, 4.3×10^{-15} atm m^3/mole
Stability: Stable to UV light
Solubility:

water (25 C), 223 mg/L (pH 5); 2240 mg/L (pH 7); 8830 mg/L (pH 9)
organic solvents g/100 mL (25 C):
acetone 0.00119
n-hexane <0.00001
acetonitrile 0.00073
methanol 0.00026
dichloromethane 0.00275
xylene 0.0001
ethanol 0.00009
ethyl acetate 0.00026
methylene chloride 0.00275

pK_a: 4.0 (25 C) (weak acid) (4)
K_{ow}: 1.6 (pH 5); 0.02 (pH 7); 0.01 (pH 9)

HERBICIDAL USE

Thifensulfuron can be applied POST at 10.5-17.5 g ai/ha in package-mix combination with tribenuron for control of many annual broadleaf weeds including kochia, wild buckwheat, and wild mustard in wheat and barley. It also can be applied POST at 4.4 g ai/ha for control of certain broadleaf weeds such as wild mustard and redroot pigweed in soybeans. A nonionic surfactant is required for maximum efficacy.

USE PRECAUTIONS

Fire hazard: All formulated products are dry and non-flammable.
Corrosiveness: All formulated products are non-corrosive.
Storage stability: Technical and formulated products are stable.
Cleaning glassware/spray equipment: Residues in spray equipment may redissolve in subsequent loads and injure susceptible crops, particularly when the herbicide used after thifensulfuron-methyl is mixed with an oil adjuvant.
Emergency exposure: Flush eyes with water for 15 min. Get medical attention if irritation persists.
Incompatibilities: Thifensulfuron-methyl applied as a tank mix with certain organophosphate insecticides or within a few days of the insecticide application can injure thifensulfuron-tolerant crops; no other tank-mix incompatibilities are known.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth of treated plants is inhibited within hr after application, but injury symptoms usually appear >1-2 wk later. Meristematic areas gradually become chlorotic and necrotic, followed by a general foliar chlorosis and necrosis.
Absorption/translocation: Rapidly absorbed by foliage and roots and translocates extensively in xylem and phloem after foliar applications with accumulation in meristematic areas.
Metabolism in plants: Soybeans rapidly deesterify thifensulfuron-methyl to the non-phytotoxic thifensulfuron acid (2). Wheat metabolized thifensulfuron-methyl with a half-life of 3-4 h, producing the deesterified free acid as the major metabolite with smaller amounts of the *O*-demethylated metabolite and sulfonylurea bridge cleavage yielding the thiophene sulfonamide and triazine amine (3). Susceptible weed species metabolize thifensulfuron slowly or not at all.
Non-herbicidal biological properties: None known

BEHAVIOR IN SOIL

Sorption:

K_{oc}: Average is 45 mL/g at pH 7 (6)
K_d: 0.08-1.38 mL/g for a silt loam soil (6)

Transformation: Degraded by microbes and by non-microbial hydrolysis. Half-life often is <1 wk.

Persistence: Average field half-life is 12 d (6), ranging from 2-6 d under aerobic and 7-28 d under anaerobic conditions.
Mobility: Highly mobile on soil thin-layer chrometography plates.
Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade thifensulfuron-methyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.7 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate (reversible within 1 d)

PINNACLE: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, mouse: NOEL 7500 mg/kg

90-d dietary, rat: NOEL male 100 mg/kg; body weight effects at 2500 and 7500 mg/kg

90-d dietary, dog: NOEL male 1500 mg/kg, female 7500 mg/kg

Chronic toxicity:

18-mo dietary, mouse: NOEL 7500 mg/kg; not oncogenic

24-mo dietary, rat: NOEL 25 mg/kg; not oncogenic; effects on body weight at 2500 mg/kg and serum sodium at 500 mg/kg

12-mo dietary, dog: NOEL 750 mg/kg; body and liver weight effects at 7500 mg/kg

Teratogenicity:

Rat: NOEL 200 mg/kg/d; not teratogenic; fetotoxic at 800 mg/kg/d

Rabbit: NOEL 200 mg/kg/d; not teratogenic; maternal toxicity at 650 mg/kg/d

Reproduction:

Rat: NOEL 2500 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: *In vivo* cytogenetics, negative; Mouse micronucleus, negative; *In vitro* test, negative

DNA damage/repair: Rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >2510 mg/kg, 8-d dietary LC_{50}, >5620 mg/kg; Earthworm LC_{50} in soil, >2000 mg/kg; Honey bee LD_{50}, >12.5 µg/bee; Daphnia 48-h LC_{50}, 470 mg/L; Bluegill sunfish 96-h LC_{50}, >100 mg/L; Rainbow trout 96-h LC_{50}, >250 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA
Purification of technical: NA
Analytical methods: Product and residue analysis by HPLC

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Arysta LifeScience; DuPont Crop Protection

thiobencarb

CAS #: 28249-77-6 **8$^{(N)}$**

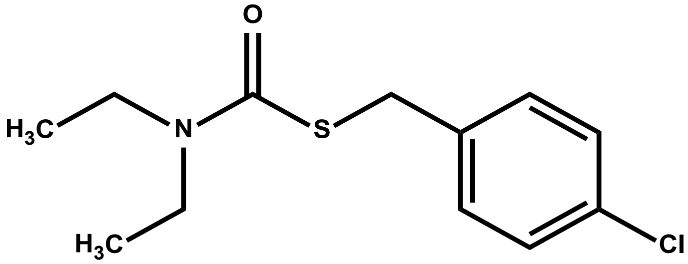
S-[(4-chlorophenyl)methyl]diethylcarbamothioate

NOMENCLATURE

Common name: thiobencarb (ANSI, BSI, ISO, WSSA)
Other name(s): benthiocarb; thiobencarbe; B-3015; *S*-4-chlorobenzyl diethylthiocarbamate (IUPAC); *S*-4-chlorobenzyl diethyl(thiocarbamate) (IUPAC); *S*-(4-chlorobenzyl) *N*,*N*-diethylthiolcarbamate
Trade name(s): ABOLISH® 8 EC; BENCARB; BOLERO® 15 G; BOLERO® 8 EC; JUPITER; SATURN 90; SATURNO; TIBOSA; VEGFRU SATURN
Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
thiobencarb



Molecular formula: $C_{12}H_{16}ClNOS$
Molecular weight: 257.78 g/mole
Description: Light yellow or brownish yellow liquid
Density: 1.14-1.18 g/mL (20 C)
Melting point: 3.3 C
Boiling point: 126-129 C (1.07 Pa)
Vapor pressure: 1.97 x 10^{-4} Pa (20 C)
Stability: Stable
Solubility:
water 30 mg/L (25 C)
organic solvents (25 C):
acetone soluble
ethanol soluble
xylene soluble
pK_a: None (non-ionizable)
K_{ow}: 2630

HERBICIDAL USE

Thiobencarb can be applied PRE or early POST at 3.4-4.5 kg ai/ha in rice. Thiobencarb controls certain grasses, rushes, sedges, and broadleaf weeds including barnyardgrass, sprangletop, junglerice, broadleaf signalgrass, spikerush, flatsedge, northern jointvetch, and dayflower.

USE PRECAUTIONS

Fire hazard: Moderate for 8EC products; flash point is 78 C
Corrosiveness: Relatively non-corrosive
Storage stability: All formulated products are stable
Cleaning glassware/spray equipment: NA
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)
Symptomology: NA
Absorption/translocation: Absorption in emerging rice seedlings is most rapid in the mesocotyl, with slower absorption occurring in the coleoptile, root, and first leaf. Thiobencarb translocates upward.
Metabolism in plants: Metabolized completely in rice. Residues in grain, hulls, and straw were 4-chlorobenzyl methylsulfone and 4-chlorobenzoic acid.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Rapidly and strongly adsorbed to soil. With soil thin-layer chromatography techniques, the Rf was ~0.1 for Stockton adobe and Oakley sandy loam.
K_{oc}: Ranges from 380-3017 mL/g in rice soils
Transformation:
Photodegradation: Can be lost from aqueous solution by photodecomposition.
Other degradation: Primarily degraded by microbes
Persistence: Moderate field residual under most conditions.
Lab experiments: Half-life ranges from 30-90 d under aerobic conditions and >1 yr under anaerobic conditions.
Mobility: Not readily leached
Volatilization: Volatilizes from aqueous solution, but losses are minimal after adsorption to soil.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade thiobencarb unless otherwise indicated.

Acute toxicity:
Oral LD_{50} rat, 1033-1130 mg/kg, mouse 2745 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 1-h inhalation LC_{50} rat, >3 mg/L; Skin irritation rabbit, mild; Skin sensitization, NA; Eye irritation rabbit, moderate, clearing in 7 d
Subchronic toxicity:
90-d dietary, rat: NOEL 660 mg/kg
Chronic toxicity:
18-mo dietary, mouse: NOEL 25 mg/kg/d; not oncogenic
24-mo dietary, rat: NOEL 1 mg/kg/d; not oncogenic
12-mo dietary, dog: NOEL 1 mg/kg/d
Teratogenicity:
Rat: NOEL 25 mg/kg/d; not teratogenic
Rabbit: NOEL 100 mg/kg/d; not teratogenic
Reproduction:
Rat: NOEL <2 mg/kg/d
Mutagenicity: NA
Wildlife:
Bobwhite quail oral LD_{50}, >7800 mg/kg; 8-d dietary LC_{50},

>5000 mg/kg; Mallard duck oral LD_{50}, >10,000 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Hen oral LD_{50}, 2629 mg/kg; Bluegill sunfish 96-h LC_{50}, 1.6-3.4 mg/L; Carp 48-h LC_{50}, 3.6 mg/L; Channel catfish 96-h LC_{50}, 2.3-6 mg/L; Rainbow trout 96-h LC_{50}, 1.05 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Residues are determined using GLC with electron capture or flame photometric detection.

Historical: Introduced in Japan in 1969 by Kumiai Chemical Industry Co. Ltd. and in the U.S. by Chevron Chemical Company; British patent 1,259,471, Japanese patent 65,740, and U.S. patent 3,582,314.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Valent

Reference(s):

1. Casida, J. E. et al. 1974. Science 184:573.
2. Fuerst, E. P. 1987. Weed Technol. 1:270-277.
3. Gronwald, J. W. 1991. Weed Sci. 39:435.
4. Prakash, T. R. et al. 1989. Weed Res. 19:427.

topramezone

CAS #: 210631-68-8

$27^{(F_2)}$

[3-(4,5-dihydro-3-isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl] (5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone

NOMENCLATURE

Common name: topramezone

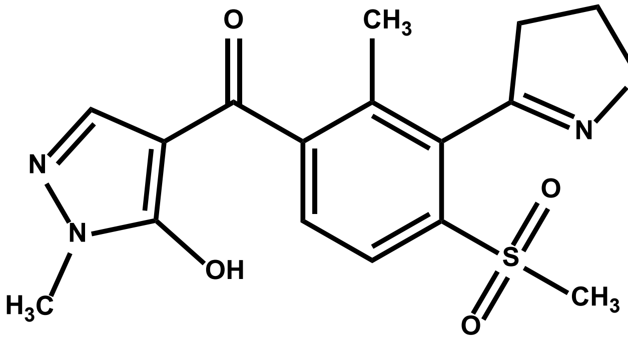
Other name(s): BAS 670H; [3-(4,5-dihyro-1,2-oxazol-3-yl)-4-mesyl-o-tolyl](5-hydroxy-1-methylpyrazol-4-yl)methanone (IUPAC)

Trade name(s): ARMEZON™; FREQUENCY™; IMPACT®; PYLEX™

Chemical family: benzoylpyrazole; pyrazolone

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure: topramezone



Molecular formula: $C_{16}H_{17}N_3O_5S$

Molecular weight: 363.39 g/mole

Description: White crystalline solid

Density: 1.4 g/mL (25 C)

Melting point: 212 C

Boiling point: NA

Vapor pressure: 1×10^{-12} Pa (20 C)

Stability: Stable in sterile aqueous solution.

Solubility: 0.69 mg/L (pH 7, 20 C) in water
water: 15 g/L (20 C)
organic solvents (g/L at 99.9% purity and 20 C);
dichloromethane 25-29
acetone <10
ethylacetate <10
DMF 114-113
acetonitrile <10
toluene <10

pK_a: 4.06 (20 C)

K_{ow}: log K_{ow} = 1.52

HERBICIDAL USE

Postemergence herbicide at a rate range of 12-25 g ai/ha for annual broadleaf and grass weed control in corn. Topramezone is also used at 100 g ai/ha for preemergence and postemergence weed control in conifer plantations and noncropland areas such as railroad, utility, highway, and pipeline rights-of-way highway guardrails, delineators, and sign posts; utility substations, petroleum tank farms, pumping installations, farmyards and around farm buildings; fence rows, storage areas, airports, and nonirrigation ditchbanks. Topramezone is also registered for use in certain turfgrasses. Postemergence applications of topramezone require the addition of an adjuvant to achieve optimum weed control.

USE PRECAUTIONS

Fire hazard: Formulated product is non-flammable

Corrosiveness: Non-corrosive

Storage stability: Keep container tightly closed in a cool, dry place.

Cleaning glassware/spray equipment: NA

Emergency exposure: On ingestion, do not induce vomiting. Dilute swallowed product with large amounts of water. On eye contact, flush with water for at least 15 minutes. On skin contact, flush with water for at least 15 minutes. On inhalation, move victim to fresh air.

Incompatibilities: Avoid strong bases and oxidizers.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of the enzyme 4-hydroxyphenyl-pyruvate dioxygenase (4-HPPD) affecting carotenoid biosynthesis. (more details on page 15)

Symptomology: Bleaching chlorosis of leaf tissue.

Absorption/translocation: Readily absorbed into roots and leaves.

Metabolism in plants: Rapidly metabolized in plants.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: HPPD-inhibitor resistant Amaranthus palmeri and A. tuberculatus have been documented. The A. tuberculatus biotype discovered in Illinois that was resistant to mesotrione and other HPPD herbicides was found to metabolize mesotrione rapidly via P450 activity.

BEHAVIOR IN SOIL

Sorption:

K_{oc}: 22.3 to 172.4 mL/g

Transformation:

Photodegradation: DT_{50} is 78 d in soil, 72 d in water

Other degradation: Aerobic soil degradation.

Persistence: DT_{50} is 14 d in soil in field.

Mobility: Residues confined mainly to top layer of soil.

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade topramezone unless otherwise indicated.

Acute toxicity:

Oral LD_{50}: rat >2000 mg/kg; Dermal LD_{50}: rat >2000 mg/kg, LC_{50} (4h) inhalation rat >5.4 mg/L; Slight skin and eye irritant (rabbit); not a skin sensitizer (guinea pig)

Subchronic toxicity: NA

Chronic toxicity:

24-mo dietary, rat: Thyroid follicular cell ademas

Teratogenicity:

Rat: NOEL 0.5 mg/kg/day

Reproduction: NA

Mutagenicity: NA

Wildlife:

Mallard ducks, oral LD_{50} >5000 mg/kg; bobwhite quail, >5000 mg/kg; honey bee, LD_{50} (contact) >100 μg/bee; rainbow trout, LC_{50} 97.4 mg/L, bluegill sunfish, 239 mg/L; Daphnia magna, EC_{50} >100 mg/L

Use classification: No restricted use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Discovered by BASF AG; first sold in the United States and Canada by Amvac Chemical Corporation under license from BASF.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Amvac; BASF

Reference(s):

1. USEPA. 2005. Pesticide Fact Sheet: Topramezone. Office of Prevention, Pesticides, and Toxic Substances. 7 pp.
2. Grossmann K. and T. Ehrhardt. 2007. Pest Manag. Sci, 63:429-439.

tralkoxydim

CAS #: 87820-88-0 $1^{(A)}$

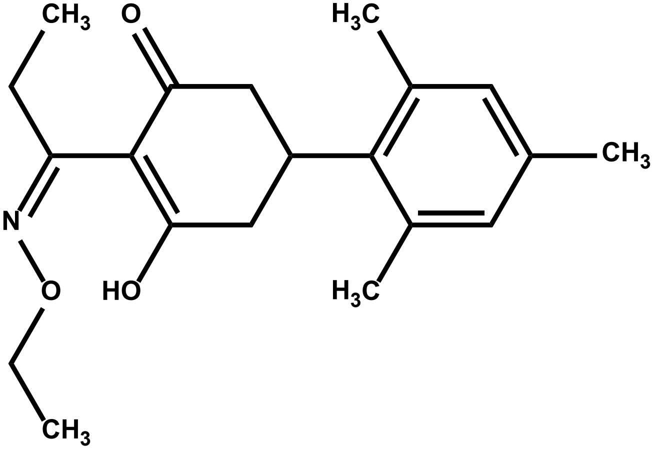
2-[1-(ethoxyimino)propyl]-3-hydroxy-5-(2,4,6-trimethylphenyl)-2-cyclohexen-1-one

NOMENCLATURE

Common name: tralkoxydim (ISO 1750 approved)
Other name(s): (RS)-2-[(EZ)-1-(ethoxyimino)propyl]-3-hydroxy-5-mesitylcyclohex-2-en-1-one
Trade name(s): ACHIEVE® ;GRASP®
Chemical family: alkylketone; cyclohexanedione; cyclohexanedione oxime; cyclohexenone; cyclohexene oxime

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:tralkoxydim



Molecular formula: $C_{20}H_{27}NO_3$
Molecular weight: 329.4 g/mole
Description: Colorless, odorless solid
Density: 1.16 g/mL (25 C)
Melting point: 106 C
Boiling point: NA
Vapor pressure: 4.2 x 10^{-7} Pa (20); 4.2 x 10^{-5} Pa (50 C); 2.13 x 10^{-3} Pa (80 C)
Stability: NA
Solubility:
water (20 C, pH 5) 6 mg/L; 6.7 mg/L (20 C, pH 6.5); 8850 mg/L (20 C, pH 9)
organic g/100 mL (24 C)

acetone 89	hexane 18
ethyl acetate 110	methanol 25
toluene 213	dichloromethane >500

pK_a: 4.3 (25 C) (weak acid)
K_{ow}: log K_{ow} =2.1 (20 C)

HERBICIDAL USE

Post control of Avena spp. and other grass weeds (Lolium spp., Setaria viridis, Phalaris spp., Alopecurus myosuroides and Apera spica-venti) in wheat and barley at 150-3400 g/ha.

USE PRECAUTIONS

Fire hazard: Can form flammable dust clouds which can easily ignite
Corrosiveness: NA
Storage stability: Stable at ambient temperatures
Emergency exposure: If ingested, was mouth out with water, do not induce vomiting. Seek medical advise. On eye contact, irrigate eye for 15 min with water/eyewash and seek medical help.
Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of acetyl CoA carboxylase (ACCase) (more details of page 12)
Symptomology: Growth ceases soon after application with young and actively growing tissues affected first. Youngest leaves turn chlorotic followed by necrosis. Complete necrosis of the plant generally occurs 10-14 d after application.
Absorption/translocation: Absorbed by leaves and translocated acropetally in the phloem to the growing points.
Metabolism in plants: Degrades rapidly in crops
Non-herbicidal biological properties: NA
Mechanism of resistance in weeds: Similar to other ACCase resistant weeds.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: 30-300 mL/g; stronger adsorption in low pH soils
Transformation:
Photodegradation: Susceptible to soil surface photolysis and aqueous photolysis
Other degradation: Primarily microbial degrada- tion
Persistence: NA
Mobility: Rapid degradation ensures low mobility
Volatilization: Low volatility

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade tralkoxydim unless otherwise indicated
Acute toxicity:
LD_{50} male rat, 1258 mg/kg, female rat, 934 mg/kg, male mice, 1231 mg/kg, female mice, 1100 mg/kg, male rabbits, >519 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; Skin and eye irritation rabbit, mild; guinea pig, none
Subchronic toxicity:
90-d dietary, rat: 20.5 mg/kg
90-d dietary, dog: 0.5 mg/kg body weight daily
Chronic toxicity:
18-mo dietary, mouse/hamster: NOAEL 5 mg/kg bw/d
24-mo dietary, rat: NOAEL 23-30 mg/kg bw/d
12-mo dietary, dog: NOEL 0.5 mg/kg bw/d
Teratogenicity: Rat: NOAEL 30 mg/kg/d – effects not seen below maternal toxicityteratogenic to rats
Rabbit: Non teratogenic
Reproduction:
No adverse reproductive effects

Mutagenicity:

Non-mutagenic in standard tests

Wildlife:

Mallard duck LD_{50}, >3020 mg/kg, partridges, 4430 mg/kg; LC_{50} (5d) mallard ducks, > 7400 mg/kg, quail, 6237 mg/kg diet; LC_{50} (96h) mirror carp, > 8.2 mg/kg; bluegill sunfish, > 6.1 mg/L; rainbow trout, 7.2 mg/L; Daphnia EC_{50} (48h), > 175 mg/L; bees LD_{50} (contact), >0.1 mg/bee, oral 0.054 mg/bee

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: Herbicide introduced by ICI (now Syngenta Crop Protection) and marketed in 1986

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

triallate

CAS #: 2305-17-5 **8$^{(N)}$**

S-(2,3,3-trichloro-2-propenyl)bis(1-methylethyl) carbamothioate

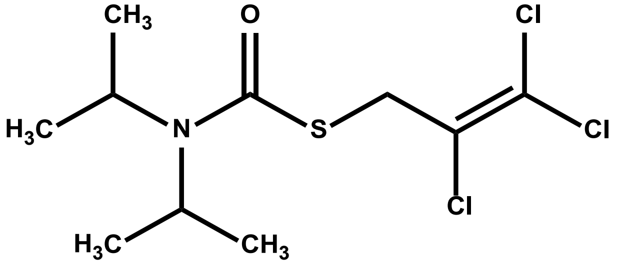
NOMENCLATURE

Common name: triallate (ISO, WSSA)
Other name(s): CP-23426;TDTC; *S*-2,3,3-trichloroallyl diisopropyl(thiocarbamate) (IUPAC); *S*-(2,3,3-trichloroallyl) diisopropylthio-carbamate (IUPAC)
Trade name(s): BUCKLE®; FAR-GO®, AVADEX®
Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical Structure

triallate



Molecular formula: $C_{10}H_{16}Cl_3NOS$
Molecular weight: 304.66 g/mole
Description: Amber-colored, oily liquid
Density: 1.27 g/mL (25/15.6˚C)
Melting point: 29-30˚C
Boiling point: 117˚ C (40 Pa); 136˚C (133 Pa)
Vapor pressure: 1.1 x10^{-4}mmHg (25˚C)
Stability: Stable to UV light; decomposes at >200˚C; hydrolyzed by strong acid and alkali
Solubility:
  water 4 ppm (20-25˚C)
  organic solvents (25˚C):
    miscible in acetone, benzene, ether, ethanol, ethyl acetate, heptane, methyl chloride, n-octanol, toluene
pK_a: None (non-ionizable)
K_{ow}: log K_{ow} = 4.54

HERBICIDAL USE

Triallate can be applied as follows: PPI or post-plant incorporated at 1.4-1.7 kg ai/ha in winter wheat, winter barley, spring barley, triticale, lentils, and peas; in the fall at 1.4-1.7 kg ai/ha in spring wheat and durum and sugar beets; PPI or post-plant incorporated at 1.1-1.4 kg ai/ha in spring wheat and durum and sugar beets; and PPI, post-plant incorporated, or in the fall at 1.1-1.7 kg ai/ha in spring barley. Triallate usually requires two incorporation passes soon after application to ensure minimal volatilization losses, although triallate applied in the fall for a spring-seeded crop can be incorporated once in the fall and again in the spring. Certain granule formulations allow application in late fall with no incorporation until spring, but only where substantial crop residue is present. Triallate controls wild oats and suppresses winter annual *Bromus* spp. Please read label for specific instructions on each crop use.

USE PRECAUTIONS

Fire hazard: FAR-GO EC is flammable; flash point is 48˚C.
Corrosiveness: Corrosive to many metals; stored or shipped at room temperature in phenolic-resin lined tanks or drums.
Storage stability: Stable indefinitely
Emergency exposure: Wash skin with soap and water. Flush eyes with water for 15 min; get medical attention. If ingested, contact a poison control center or physician immediately. Consult product labels for full directions.
Incompatibilities: Compatible with most liquid fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)
Absorption/translocation: Primarily absorbed by the emerging grass coleoptile, less so by roots.
Metabolism in plants: Triallate is metabolized
Non-herbicidal biological properties: None known

BEHAVIOR IN SOIL

Sorption:
K_{oc}: Average is 2400 mL/g
Transformation:
  Photodegradation: Negligible losses
  Other degradation: Triallate is microbially degraded in soil
Persistence: Average field half-life is 68 d. Triallate residues do not persist long enough to injure crops the following season.
Mobility: Not mobile in high OM soils
Volatilization: Losses are substantial when applied to warm soils and not properly incorporated.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 3612 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >5.3 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

FAR-GO: Oral LD_{50} rat, 2193 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50} rat, >5.2 mg/L; Skin irritation rabbit, slight; Eye irritation rabbit, moderate

Wildlife:

Bobwhite quail oral LD_{50}, 2251 mg/kg; 5-d dietary LC_{50}, >5620 mg/kg; Mallard duck 5-d dietary LC_{50}, >5620 mg/kg; Honey bee topical LD_{50}, >25 µg/bee; Daphnia 48-h LC_{50}, 0.43 mg/L; Bluegill sunfish 96-h LC_{50}, 1.3 mg/L;

Rainbow trout 96-h LC_{50}, 1.2 mg/L; Algae 96-h EC_{50}, 0.12 mg/L

FAR-GO: Bobwhite quail 8-d dietary LC_{50}, >5620 mg/kg; Daphnia 48-h LC_{50}, 0.57 mg/L; Bluegill sunfish 96-h LC_{50}, 2.4 mg/L; Rainbow trout 96-h LC_{50}, 1.5 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: First reported in 1962 (3). Introduced by Stauffer Chemical Company. U.S. patent 2,913,327.

MANUFACTURER(S) AND INFORMATION SOURCES:

Manufacturer(s): Gowan Company

Source(s): Gowan Company

Reference(s):

1. California Dept. of Pesticide Regulation Public Report 2007-5. Triallate. Tracking ID# 215144.
2. Environmental Protection Agency (EPA). Reregistration Eligibility Decision (RED) for Triallate. EPA 738-R-00-021. March 2001.

triasulfuron

CAS #: 82097-50-5

2$^{(B)}$

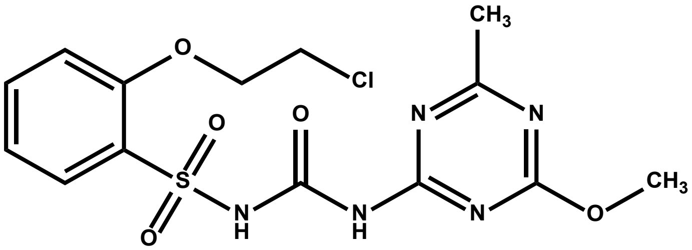
2-(2-chloroethoxy)-*N*-[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulfonamide

NOMENCLATURE

Common name: triasulfuron (ANSI, BSI, ISO, WSSA)
Other name(s): CGA-131036; 2-(2-chloroethoxy) phenylsulfonyl]-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl) urea (IUPAC); *N*-(6-methoxy-4-methyl-1,3,5-triazin-2-yl-amino-carbonyl)-2-(2-chloroethoxy)-benzenesulfonamide
Trade name(s): AMBER®; LOGRAN; RAVE®
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
triasulfuron



Molecular formula: $C_{14}H_{16}ClN_5O_5S$
Molecular weight: 401.82 g/mole
Description: Colorless crystalline solid, odorless
Density: 1.5 g/mL (20 C)
Melting point: 186 C
Boiling point: NA
Vapor pressure: 2×10^{-6} Pa (25 C); Henry's Law constant, $<9.7 \times 10^{-12}$ atm m^3/mole
Stability: Hydrolyzes at pH 3 and 50 C (half-life = 2 h); partially degrades just below 186 C and degrades at >186 C
Solubility:
water (25 C), 32 mg/L (pH 5); 815 mg/L (pH 7); 13,500 mg/L (pH 9)
organic solvents g/100 mL (25 C):

acetone 1.4	methanol 0.34
cyclohexanone 1.7	methylene chloride 3.6
ethanol 0.043	*n*-octanol 0.013
ethyl acetate 0.43	toluene 0.03
n-hexane 0.000004	xylene 0.017

pK$_a$: 4.64 (weak acid)
K$_{ow}$: 0.31 (25 C)

HERBICIDAL USE

Triasulfuron can be applied POST at 15-30 g ai/ha in wheat, barley, and fallow, or PRE in wheat for control of many annual broadleaf weeds including mustard spp., kochia, pigweed spp., common ragweed, and common sunflower. A surfactant is required for maximum POST efficacy.

USE PRECAUTIONS

Fire hazard: The product AMBER is non-flammable.
Corrosiveness: The product AMBER is non-corrosive.
Storage stability: Shelf life of AMBER is estimated to be >6 mo at room temperature. Light or moisture may shorten shelf life.

Cleaning glassware/spray equipment: Wash glassware and spray equipment with a water/ammonia solution, and triple rinse with water. Clean nozzles and screens separately
Emergency exposure: May irritate eyes. If ingested, induce vomiting or lavage stomach. No specific antidote is available but a slurry of activated charcoal may help adsorb ingested triasulfuron
Incompatibilities: Crop injury may result if malathion or certain other organophosphate insecticides are tank mixed or applied sequentially with triasulfuron. Compatible with most other pesticides and fertilizers

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth is rapidly inhibited in susceptible species, resulting in stunted plants. Foliar chlorosis begins to appear within 6-10 d, followed by chlorosis and necrosis of the growing point of broadleafs, and foliar necrosis. Veins on the underside of leaves are discolored, often reddish purple. Root growth inhibition sometimes occurs. Complete plant death may require 15-30 d.
Absorption/translocation: Readily absorbed by both foliage and roots, and translocates extensively in xylem and phloem. When applied to leaves, triasulfuron translocates to shoot growing points and at moderate levels to the roots. Root-absorbed triasulfuron translocates efficiently to all parts of the shoots, including meristematic areas.
Metabolism in plants: Wheat rapidly detoxifies triasulfuron by hydroxylation of the phenyl ring followed by conjugation with glucose. Hydrolytic cleavage of the urea bridge also occurs but at a slower rate, producing a benzenesulfonamide derivative, a triazine amine derivative, and CO_2.
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Sulfonylurea-resistant weed biotypes selected in the field by chlorsulfuron use typically are resistant to triasulfuron. The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: Low adsorption to clay and soil colloids
K$_{oc}$ and K$_d$: K$_{oc}$ 191 mL/g and K$_d$ 0.76 mL/g for a loamy sand with 0.8% OM, 9% clay, and pH 7.8; K$_{oc}$ 73.4 mL/g and K$_d$ 1.14 mL/g for a sandy loam with 3.1% OM, 7% clay, and pH 7.5; K$_{oc}$ 51.6 mL/g and K$_d$ 1.16 mL/g for a silt loam with 4.5% OM, 13% clay, and pH 7.2; K$_{oc}$ 65.2 mL/g and K$_d$ 0.62 mL/g for a silty clay loam with 1.9% OM, 34%

clay, and pH 7.1.

Transformation:

Photodegradation: Half-life was 87 d in water at pH 9 and 22-26 C. Half-life on a sandy loam at 25 C under natural light ranged from 69-139 d

Other degradation: Hydrolysis half-life in sterile water at pH 5 was 31-32 d. Half-life ranged from 69-139 d in separate 1-yr aerobic studies at 25 C in a sandy loam or a silt loam, with the sulfonylurea bridge cleavage product 2-(2-chloroethoxy) benzenesulfonamide as the major metabolite. Half-life was 112 d in a 1-yr anaerobic study at 25 C in a sandy loam, producing the same major metabolite. Biological degradation is a major contributor to soil dissipation at high soil pH where non-microbial hydrolysis rate is slow. At lower pH, hydrolysis is a major contributor.

Persistence: Somewhat persistent. Triasulfuron residues can persist in soil long enough to injure certain broadleaf crops 1-3 yr after application.

Field experiments: Half-lives in bare ground dissipation studies sampling 0-15 cm: 20-25 d for a sandy loam with 0.8% OM and pH 5.8 in California; 11-20 d for a silt loam with 2% OM and pH 6.2 in Kansas; 9.5-26 d for a clay loam with 1.8% OM and pH 7.4 in Mississippi; 19-95 d for a silt loam with 2.5% OM and pH 5.5 in New York. Half-life can vary substantially with environmental conditions.

Mobility: In field experiments conducted in wheat grown in Kansas and North Dakota, no quantifiable triasulfuron residues (LOD = 0.5-1 µg/kg) were found below 30 cm.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade triasulfuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rat, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.2 mg/L; Skin irritation rabbit, slight; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

AMBER: Oral LD_{50} rat, >5050 mg/kg; Dermal LD_{50} rabbit, >2010 mg/kg; 4-h inhalation LC_{50} rat, >2.3 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, mouse: NOEL <10,000 mg/kg; liver effects at >10,000 mg/kg

90-d dietary, rat: NOEL 14.5 mg/kg/d; kidney effects and reduced body weight gain at >10,000 mg/kg, with secondary hematological and blood chemistry changes

90-d dietary, dog: NOEL 3 mg/kg/d; liver, kidney, and spleen effects at $\geq$5000 mg/kg

21-d dermal, rabbit: NOEL 100 mg/kg/d; clinical signs of toxicity at 1000 mg/kg/d

Chronic toxicity:18-mo dietary, mouse: NOEL 1.2 mg/kg/; not carcinogenic at $\leq$10,000 mg/kg (highest dose tested); liver effects at ≥1000 mg/kg

24-mo dietary, rat: NOEL 10 mg/kg; not carcinogenic at $\leq$6000 mg/kg (highest dose tested; liver effects at $\geq$1000 mg/kg

12-mo dietary, dog: NOEL 33 mg/kg/d; liver, kidney, and spleen effects at 5000 mg/kg (highest dose tested)

Teratogenicity:

Rat: NOEL maternal 100 mg/kg/d, developmental 300 mg/kg/d; not teratogenic

Rabbit: NOEL maternal 120 mg/kg/d, developmental 240 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 2500 mg/kg; NOEL maternal 1000 ppm, developmental 5000 mg/kg; no reproductive effects at 5000 mg/kg (highest dose tested)

Mutagenicity:

Gene mutation: Ames test, negative; Mouse lymphoma (L51784/TK+1), negative; *S. cerevisiae*, negative

Structural chromosome aberration: CHO, negative; Mouse micronucleus, negative; Chinese hamster/nucleus anomaly, negative

DNA damage/repair: Rat hepatocytes, negative; Human fibroblasts, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck oral LD_{50}, >2150 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Honey bee oral LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, >100 mg/L; Bluegill sunfish 96-h LC_{50}, >100mg/L; Rainbow trout 96-h LC_{50}, >100 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: A multi-step synthesis beginning with chlorophenol and culminating with the coupling of an amino triazine with a benzene-sulfonyl isocyanate.

Purification of technical: Suspension in an acidic water/alcohol mixture, followed by filtration, water washing, and vacuum drying.

Analytical methods: Crop samples are homogenized in methanol-phosphate buffer and cleaned-up by solvent partition and solid phase extraction on a cyanopropylsilica cartridge. Residues are determined by LC using column switching. Soil samples are extracted in 1:1 methanol:carbonate buffer and cleaned-up by solvent partition and solid phase extraction. Water samples are extracted by solvent partition and determined by HPLC with UV detection. Triasulfuron is determined in technical samples and in formulations using reversed phase HPLC with UV detection at 230 nm.

Historical: Triasulfuron was synthesized by Ciba-Geigy Limited in 1981 in Basel, Switzerland, and was first used commercially on wheat in 1992. First reported in 1985 (1). U.S. patent 4,514,212 and European patent 44,808 issued April 30, 1985.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. Amrein and Gerber. 1985. Br. Crop Prot. Conf. Weeds 1:55.
2. LaRossa and Schloss. 1984. J. Biol. Chem. 259:8753.

tribenuron-methyl

CAS #: 106040-48-6 **$2^{(B)}$**

methyl 2-[[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)
methylamino]carbonyl]amino]sulfonyl]benzoate

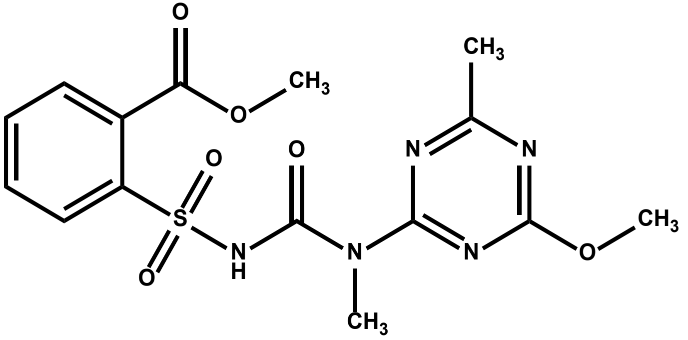
NOMENCLATURE

Common name: tribenuron-methyl (ANSI, ISO, WSSA)
Other name(s): DPX-L5300; methyl 2-[4-methoxy-6-methyl-1,3,5-triazin-2-yl) (methyl)carbamoylsulfamoyl] benzoate (IUPAC)
Trade name(s): AFFINITY®; ALLY®; CANOPY®; EXPRESS®; GRANSTAR®; HARMONY® EXTRA; HARMONY® XP; SUPREMACY®
Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

tribenuron-methyl



Molecular formula: $C_{15}H_{17}N_5O_6S$
Molecular weight: 395.39 g/mole
Description: Light brown solid
Density: NA
Melting point: 141 C
Boiling point: NA
Vapor pressure: 5.2×10^{-8} Pa (25 C); Henry's Law constant, 1.02×10^{-13} atm m^3/mole
Stability: Stable
Solubility:
water, 48 mg/L (pH 5, 25 C); 2040 mg/L (pH 7, 25 C); 18,300 mg/L (pH 9, 25 C)
organic solvents g/100 mL (25 C):
acetone 0.00438 *n*-hexane 0.0000028
acetonitrile 0.00542 methanol 0.000339
carbon tetrachloride 0.000312
ethyl acetate 0.00175
pK_a: 5.0 (weak acid)
K_{ow}: 0.36 (pH 7)

HERBICIDAL USE

Tribenuron-methyl can be applied POST at 8.8-17.5 g ai/ha in wheat and barley. When applied as the tribenuron-methyl + thifensulfuron commercial mixture (HARMONY EXTRA), tribenuron-methyl rates are 5.3-8.8 g ai/ha. Tribenuron controls many annual broadleaf weeds such as mustard spp., common lambsquarters, henbit, prickly lettuce, and kochia, and suppresses Canada thistle.
(comment: it may be good to mention about ExpressSun sunflower here)

USE PRECAUTIONS

Fire hazard: The product is dry and non-flammable.
Corrosiveness: The product is non-corrosive.
Storage stability: Stable
Cleaning glassware/spray equipment: Residues in spray equipment may redissolve in subsequent loads and injure susceptible crops, particularly when the herbicide used after tribenuron-methyl is mixed with an oil adjuvant. Thoroughly remove all residues by following labeled spray tank cleanout procedure.
Emergency exposure: May irritate eyes, nose, throat, and skin
Incompatibilities: Compatible with most broadleaf herbicides and fungicides, but antagonizes POST grass herbicides such as diclofop. Do not use adjuvants that lower spray solution pH below 3. Crop injury can occur when mixing with highly acidic liquid fertilizers or surfactants containing liquid fertilizer. Tribenuron applied as a tank mix with certain organophosphate insecticides such as malathion or within a few days of the insecticide application can injure small grains, particularly when the crop is stressed.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Growth of treated plants is inhibited within a few h after application, but susceptible weeds die 7-21 d later. Meristematic areas gradually become chlorotic and necrotic, followed by general foliar chlorosis and necrosis. Other potential symptoms include purpling (anthocyanin accumulation) of leaves, loss of leaf nyctinasty, leaf abscission, and vein discoloration.
Absorption/translocation: Rapidly absorbed by foliage and roots and translocated throughout the plant via xylem and phloem, but primarily the phloem.
Metabolism in plants: In tolerant plants, tribenuron is rapidly undergoes oxidative reactions that are mediated by cytochrome P-450 enyzmes (4).
Non-herbicidal biological properties: None of significant value
Mechanism of resistance in weeds: Sulfonylurea-resistant weed biotypes selected in the field by chlorsulfuron use typically are resistant to tribenuron-methyl. The mechanism of resistance is an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption:
K_{oc}: Average is 46 mL/g (pH 6.6) (1)
Transformation:
Photodegradation: Negligible losses

Other degradation: Rapidly degraded by non-microbial hydrolysis resulting in cleavage at the sulfonylurea bridge. Hydrolysis is faster in lower pH soils. Tribenuron-methyl also is rapidly degraded by microbes.

Persistence: Short residual with an average field half-life of 10 d at pH 6 (1). Any rotational crop can be planted 60 d after application.

Mobility: NA

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade tribenuron unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, mild

EXPRESS: Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate

Subchronic toxicity:

90-d dietary, rat: NOEL 100 mg/kg; body and organ weight effects

90-d dietary, dog: NOEL 500 mg/kg; body weight effect at 2500 mg/kg

Chronic toxicity:

18-mo dietary, mouse: NOEL 30 mg/kg/d; not oncogenic; body weight effect at 1500 mg/kg

24-mo dietary, rat: NOEL 25 mg/kg; mammary gland adenocarcinoma in females at 1250 mg/kg; body weight effects at 250 and 1250 mg/kg

12-mo dietary, dog: NOEL 8.2 mg/kg/d; body weight and serum creatinine effects at 1500 mg/kg

Teratogenicity:

Rat: NOEL 20 mg/kg/d; not teratogenic; maternal and fetal toxicity at 125 mg/kg/d

Rabbit: NOEL 20 mg/kg/d; not teratogenic; maternal and fetal toxicity at 80 mg/kg/d

Reproduction:

Rat: NOEL 25 mg/kg; body weight effects at 250 mg/kg

Mutagenicity:

Gene mutation: Ames test, negative; CHO, negative

Structural chromosome aberration: In vivo rat bone marrow/cytogenetics, negative; Mouse micronucleus, negative; Human lymphocytes, negative

DNA damage/repair: Rat hepatocytes/UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg, 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck 8-d dietary LC_{50}, >5620 mg/kg; Earthworm LC_{50} in soil, >1200 mg/kg; Honey bee topical LD_{50}, >100 μg/bee; Daphnia 48-h LC_{50}, 720 mg/L; Bluegill sunfish 96-h LC_{50}, >1000 mg/L; Rainbow trout 96-h LC_{50}, >1000 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Product and residue analysis by HPLC

Historical: Tribenuron was first introduced in Spain in 1986 and in the U.S. as EXPRESS in 1989.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Arysta LifeScience; DuPont Crop Protection

triclopyr

[(3,5,6-trichloro-2-pyridinyl)oxy]acetic acid

CAS # Acid: 55335-06-3
Butoxyethyl ester: 81406-37-3
Triethylamine salt: 57213-69-1

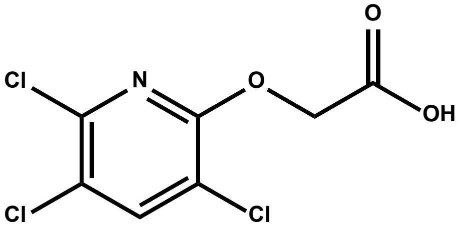
4$^{(O)}$

NOMENCLATURE

Common name: triclopyr (ANSI, BSI, ISO, WSSA)
Other name(s): DOWCO 233; 3,5,6-trichloro-2-pyridinyloxyacetic acid (IUPAC)
Trade name(s): ALLIGARE TRICLOPYR 3; ALLIGARE TRICLOPYR 4E; ALLIGARE TRICLOPYR RTU HERBICIDE; ALLIGARE EVERETT HERBICIDE; ALLIGARE PRESCOTT HERBICIDE; CANDOR HERBICIDE; CHASER TURF HERBICIDE; COOL POWER SELECTIVE HERBICIDE; CONFRONT™ F; CROSSBOW™; DOW AGROSCIENCES BRUSH AND WEED HERBICIDE; FORESTRY GARLON™ 4; FORESTRY GARLON™ XRT; GARLON™ 3A; GARLON™ 4; GARLON™ 4 ULTRA; GARLON XRT; GRANDSTAND™ R; GRASP™ XTRA HORSEPOWER™ SELECTIVE HERBICIDE;
Chemical family: pyridinecarboxylic acid; pyridine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:



Molecular formula: *Acid* $C_7H_4Cl_3NO_3$; *Butoxyethyl ester (Be ester)* $C_{13}H_{16}Cl_3NO_4$; *Triethylamine (Tea) salt* $C_{13}H_{19}Cl_3N_2O_3$
Molecular weight: *Acid* 256.47 g/mole; *Be ester* 356.63 g/mole; *Tea salt* 357.66 g/mole
Description: Fluffy white solid
Density: 1.85 g/mL
Melting point: 148-150 C
Boiling point: Decomposes before boiling
Vapor pressure: 1.6 x 10^{-4} Pa (25 C); 7 x 10^{-4} Pa (40 C); 1 x 10^{-3} Pa (50 C); 1.3 x 10^{-2} Pa (70 C)
Stability: Decomposed by UV light; decomposes at 290 C. Triclopyr BEE hydrolyses readily in water; triclopyr acid is stable to hydrolysis.
Solubility:

Acid

water 430 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone 98.9
acetonitrile 12.6
benzene 2.73
chloroform 2.73
ethanol soluble
n-hexane 0.041
n-octanol 30.7
xylene 2.79

Butoxyethyl ester

water 23 mg/L (25 C) (5)

Triethylamine salt

water 2,100,000 mg/L (25 C) (5)

pK_a: 2.68 (weak acid)

K_{ow}: 2.64 (pH 5); 0.36 (pH 7); 0.11 (pH 9)

HERBICIDAL USE

Triclopyr is intended for the control of woody plants, broadleaf weeds in range and permanent grass pasture, conservation reserve program (CRP) acres (including fence rows and non-irrigation ditch banks within these areas), forests and non-crop areas including manufacturing and storage sites, rights-of-way such as electrical power lines, communication lines, pipelines, roadsides, railroads, fence rows, non-irrigation ditch banks, and around farm buildings; and applications to grazed areas, and establishment and maintenance of wildlife openings, seasonally dry wetlands. and in Christmas tree plantations. Triclopyr formulated as the TEA salt can also be used to control emerged, submerged and floating aquatic plants in aquatic sites such as ponds, lakes, reservoirs, non-irrigation canals, seasonal irrigation waters and ditches which have little or no continuous outflow, marshes and wetlands, including broadleaf and woody vegetation on banks and shores within or adjacent to these and other aquatic sites.Triclopyr can be foliar-applied at 1.12-9.1 kg ae/ha in non-crop land areas such as utility and pipeline rights-of-way, roadsides, railroads, industrial sites. In forestry sites triclopyr can be applied up to 6.8 kg ae/l and on , rangeland and permanent pastures or other grazed sites triclopyr can be applied up to 2.3 kg ae/A on except for lactating animals for which grazing is not allowed until the next growing season . It can be applied POST at 0.28-1.12 kg ae/ha in turf, and POST at 0.28-0.42 kg ae/ha in rice. Triclopyr also can be applied for site preparation or broadcast or directed-POST for conifer release depending on conifer species and stage of growth, as cut surface applications (injection frill or girdle and cut stump), and the ester formulations can be mixed with oil for basal bark or in oil:water mixtures for dormant stem treatments on small trees or brush. It controls many annual broadleaf weeds including black medic, clover spp., dandelion, ground ivy, burdock, and plantain spp., as well as many tree and brush species. Triclopyr TEA formulations require use of a non-ionic surfactant for maximum efficacy. Triclopyr TEA can be applied as either a surface or subsurface application for the control of susceptible submerged weeds including Eurasian watermilfoil in ponds, lakes, reservoirs, and in non-irrigation canals or ditches (with little or no continuous outflow) at triclopyr concentrations of 0.75 to 2.5 ppm ae in treated water. Use higher rates in the rate range in areas of greater water exchange.

USE PRECAUTIONS

Fire hazard: GARLON 4, REMEDY, and TURFLON ESTER are combustible but non-flammable with flash points of 64 C (TCC). GARLON 4 Ultra and Remedy 4 Ultra are also combustible but non-flammable with flash points >93 C.

GARLON 3A and TURFLON AMINE are non-flammable; flash points are 43 C.

Corrosiveness: Slightly corrosive to aluminum on extended exposure

Storage stability: Stable for >2 yr. Store above 2 C to prevent crystallization, or agitate before use.

Cleaning glassware/spray equipment: Detergent wash and rinse with water.

Emergency exposure: Flush eyes or skin with water. If ingested, do not induce vomiting; seek medical assistance.

Incompatibilities: Formulated products are incompatible with oxidizing substances, acid, and base.

BEHAVIOR IN PLANTS

Mechanism of Action: Not completely understood but similar to that of endogenous auxin (IAA) and other auxin-type herbicides. (more details on page 12)

Symptomology: Symptoms are typical of other auxin-type herbicides, and include epinastic bending and twisting of stems and petioles, stem swelling (particularly at nodes) and elongation, and leaf cupping and curling. Leaf shape and venation often appear abnormal. This is followed by chlorosis at the growing points, growth inhibition, wilting, and necrosis. Death of susceptible plants occurs slowly, usually within 3-5 wk. At low concentrations, young leaves may appear puckered and the tips of new leaves may develop into narrow extensions of the midrib.

Absorption: Triclopyr readily penetrates foliage, with a rain-free period of 4 h required for maximum efficacy. The butoxyethyl ester is absorbed by leaves particularly rapidly. Uptake into wheat and barley leaves was essentially complete 12 h after treatment (3). However, foliar penetration in chickweed, a susceptible species, was considerably slower and less complete than in wheat or barley.

Translocation: Rapidly transported in plants, primarily via the symplastic pathway (including the phloem), and accumulating at the growing points (4). Between 40 and 67% of triclopyr penetrating the foliage of barley, wheat, and chickweed moved out of the treated leaf within 3 d of application (3). About 3.6% of foliar-applied triclopyr accumulated in the roots of horsenettle (2). Root-absorbed triclopyr appears to translocate to shoots.

Metabolism in plants: Triclopyr esters are rapidly hydrolyzed to the triclopyr acid. While metabolism of the acid may be slow in some plants (2, 4), it appears to be rapid in others, particularly in tolerant cereals (3). Both barley and wheat metabolized at least 85% of the acid and ester forms of triclopyr by 3 d after application. Metabolites included a mixture of unidentified water-soluble sugar conjugates, as well as an aspartate conjugate and a methyl ester. In chickweed, a glutamate conjugate also was identified.

Non-herbicidal biological properties: None known

Mechanism of resistance in weeds: No known cases of resistance.

BEHAVIOR IN SOIL

Sorption: Not strongly adsorbed; varies with soil OM and clay content.

K_{oc}: Average is 35 mL/g for triclopyr acid, 20 mL/g (estimated) for the triethylamine salt and 780 mL/g for the butoxyethyl ester (5)

Transformation:

Photodegradation: Rapidly degraded; laboratory half-life is 2-6 h in water; rapidly degraded by photolysis in water with a half-life of 10 h at 25 C, producing trichloropyridinol as the major metabolite.

Other degradation: Degraded by microbes in soil.

Persistence: Triclopyr is moderately persistent with an average half-life of 30 d, ranging from 10-46 d depending on soil characteristics, moisture, and temperature.

Mobility: Field studies have not shown movement beyond 30 centimeters (11.8 inches) of the soil surface under normal weather conditions. Besides the amount of precipitation, movement of triclopyr through the soil profile depends on the organic matter content.

Volatilization: Negligible losses

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade triclopyr acid unless otherwise indicated.

Acute toxicity:

Triclopyr acid: Oral LD_{50} rat, 712 mg/kg, Dermal LD_{50} rabbit, >2000 mg/kg; inhalation LC_{50} 4.8 mg/kg; Skin irritation rabbit, non-irritatinig; Skin sensitization guinea pig, positive in concentrated solution, negative in dilute solution; Eye irritation rabbit, mild

GARLON 3A: Oral LD_{50} male rat, 2574 mg/kg; Dermal LD_{50} rabbit, >5000 mg/kg; 4-h inhalation LC_{50}, >2.6 mg/kg; Eye irritation rabbit, severe

GARLON 4: Oral LD_{50} male rat, 1581 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50}, >5.2 mg/L; Skin irritation rabbit, moderate; Skin sensitization guinea pig, positive in concentrated solution, negative in dilute solution; Eye irritation rabbit, slight

Subchronic toxicity:

90-d dietary, rat: NOEL 5 mg/kg/d; decreased body weight gain at >50 mg/kg/d and kidney effects at >20 mg/kg/d

1-yr dietary, dog: NOEL 5 mg/kg/d.

28-d immunotoxicity: rat: NOEL for systemic toxicity 10 mg/kg/d; not immunotoxic

90-d Neurotoxicity, rat: NOEL for systemic toxicity 25 mg/kg/d; not neurotoxic

Chronic toxicity:

22-mo dietary, mouse: NOEL 5.3 mg/kg/d; not oncogenic

24-mo dietary, rat: NOEL 3 mg/kg/d; not oncogenic

Teratogenicity:

Rat: NOEL 50 mg/kg/day (fetal and maternal eval.); not teratogenic

Rabbit: NOEL 75 mg/kg/day (fetal) and 25 mg/kg/day (maternal); not teratogenic

Reproduction:

Rat: NOEL 25 mg/kg/d; NOEL 5 mg/kg/d (paternal); not a selective reproductive toxin

Mutagenicity: *In vitro* and *in vivo* tests indicate no mutagenic potential

Chronic Exposure: EPA has concluded that chronic exposure to triclopyr and its metabolites from food and water will utilize 0.2% of the chronic Population Adjusted Dose (cPAD, also called the “aggregate exposure Risk Cup”) for the general U.S. population and all population subgroups. Regulatory concern is not justified until the cPAD exceeds 100%.

Wildlife:

Triclopyr acid: Bobwhite quail 8-d dietary LC_{50}, 2934 mg/kg; Japanese quail 8-d dietary LC_{50}, 3272 mg/kg; Long-term reproductive NOEC, 500 mg/kg; Mallard duck oral LD_{50}, 1698 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Long-term reproductive NOEC, 400 mg/kg; Honey bee oral LD_{50}, >100 µg/bee; topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 133 mg/L; 21-d NOEC, 48.5 mg/L; Bluegill sunfish 96-h LC_{50}, 148 mg/L; Rainbow trout 96-h LC_{50}, 117 mg/L; 28-d NOEC, 46.3 mg/L; *Pseudokirchneriella subcapitata* 96-h EC_{50},42 mg/L

Triclopyr butoxyethyl ester technical: Bobwhite quail oral LD_{50}, 735 mg/kg; 8-d dietary LC_{50}, 5401 mg/kg; Mallard duck oral LD_{50}, 4640 mg/kg; 8-d dietary LC_{50}, >5401 mg/kg; Honey bee oral LD_{50}, >110 µg/bee; topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 12.0 mg/L; Bluegill sunfish 96-h LC_{50}, 0.36 mg/L; Rainbow trout 96-h LC_{50}, 0.65 mg/L; *Pseudokirchneriella subcapitata* 96-h EC_{50}, >3.0 mg/L

Triclopyr triethylamine salt technical: Bobwhite quail 8-d dietary LC_{50}, 11,622 mg/kg; Mallard duck oral LD_{50}, 3176 mg/kg, 8-d dietary LC_{50}, >10,000 mg/kg; Honey bee topical LD_{50}, >100 µg/bee; Daphnia 48-h LC_{50}, 1496 mg/L; 21-d NOEC, 80.7 mg/L; Bluegill sunfish 96-h LC_{50}, 893 mg/L; Rainbow trout 96-h LC_{50}, 613 mg/L; Fathead minnow 96-h LC_{50}, 279 mg/L; ELS NOEC, 104 mg/L; *Pseudokirchneriella subcapitata* 96-h EC_{50}, 16.7 mg/L

Use classification: General use

SYNTHESIS ANALYTICAL METHODS

Purification of technical: Not included

Analytical methods: Residue analysis in water, soil, and leaf, and tissue samples is done by GC-MS or LC-MS/MS with limits of detection as low as 10 ug/L or ug/kg.

Historical: First reported in 1975 (1). Introduced by Dow Chemical Co.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Dow AgroSciences

Reference(s):

1. Byrd, B. C. et al. 1975. Proc. West. Soc. Weed Sci. 28:44.
2. Gorrell, R. M. et al. 1988. Weed Sci. 36:447.
3. Lewer and Owen. 1990. Pestic. Biochem. Physiol. 36:187.
4. Radosevich and Bayer. 1979. Weed Sci. 27:22.
5. Petty D.G., K.D. Getsinger,and K.B. Woodburn. 2003. J. Aquat. Plant Manage.41: 69-77
6. USA EPA Registration Eligibility Decision (RED). Triclopyr October 1998. EPA 738-R-98-011.
7. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.
8. Syracuse Environmental Research Associates, Inc. 2011. Triclopyr Human Health and Ecological Risk Assessment Final Report. SERA TR-052-25-03b. Report dated October 20, 2011. Available at: http://www.fs.fed.us/foresthealth/pesticide/risk.shtml

trietazine

6-chloro-*N,N,N′*-triethyl-1,3,5-triazine-2,4-diamine

CAS #: 1912-26-1

5$^{(C_1)}$

NOMENCLATURE

Common name: trietazine (ISO)

Other name(s): G 27901; NC 1667; 6-chloro-N^2,N^2,N^4-triethyl-1,3,5-triazine-2,4-diamine (IUPAC)

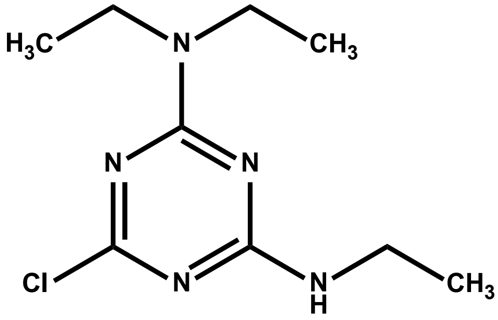
Trade name(s): REMTAL®

Chemical family: chloro-*s*-triazine; chlorotriazine; *s*-triazine; triazine

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

trietazine



Molecular formula: $C_9H_{16}ClN_5$

Molecular weight: 229.71 g/mole

Description: Colorless crystals

Density: NA

Melting point: 100-101 C

Boiling point: NA

Vapor pressure: 8.9×10^{-3} Pa (20 C)

Stability: Stable in neutral media; hydrolyzed by strong acids and alkalis

Solubility:

water, 20 mg/L (25 C)

acetone 170 g/L	benzene 200 g/L
chloroform >500 g/L	ethanol 30 g/L.

pK_a: 1.88 (weak base)

K_{ow}: log K_{ow} = 3.34

HERBICIDAL USE

Trietazine is a selective herbicide used with linuron for weed control in potatoes, with simazine in peas, and with terbutryn in potatoes, peas and field beans at 1.6 to 4.5 kg a.i./ha according to crop and soil characteristics. Not marketed in the U.S.

USE PRECAUTIONS

Fire hazard: NA

Corrosiveness: Non-corrosive

Storage stability: NA

Emergency exposure: NA

Incompatibilities: NA

BEHAVIOR IN PLANTS

Mechanism of action: Inhibits photosynthesis at photosystem II (PS II) (more details on page 13)

Symptomology: Chlorosis followed by necrosis of affected plant tissue

Absorption/translocation: Absorbed by roots and leaves; predominately xylem translocated.

Metabolism in plants: NA

Mechanism of resistance in weeds: Altered target site

BEHAVIOR IN SOIL

Transformation:

Photodegradation: NA

Other degradation: Microbial degradation of trietazine yields chlorine atom cleavage to produce hydroxytriazine compounds which are conjugated with amino acids.

Persistence:

Field experiments: NA

Lab experiments: NA

Volatilization: Negligible

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade trietazine unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, 494-841 mg/kg; Dermal LD_{50} rat, >600 mg/kg; non-irritating to skin (rats)

Subchronic toxicity:

90-d dietary, rat: NOEL 16 mg/kg diet

Wildlife:

Acute oral LD_{50} for quail, 800 mg/kg. LC_{50} (24 h) for guppies, 5.5 mg/l; non-toxic to honeybees

Use classification: WHO class III

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: NA

Historical: NA

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Bayer CropScience

trifloxysulfuron

CAS # Acid: 145099-21-4
Na salt: 199119-58-9

$2^{(B)}$

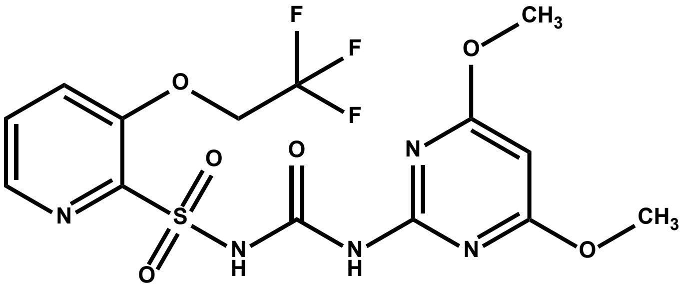
N-[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]-3-(2,2,2-trifluoroethoxy)-2-pyridinesulfonamide

NOMENCLATURE

Common name: trifloxysulfuron (BSI, pa ISO)
Other name(s): CGA-362 622; 1-(4,6-dimethoxy-pyrimidin-2-yl)-3-[3-(2,2,2-trifluoroethoxy)-2-pyridylsulfonyl]urea (IUPAC)
Trade name(s): ENFIELD™; ENVOKE™; KRISMAT™; MONUMENT™
Chemical family: pyrimidinylsulfonylurea; sulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
trifloxysulfuron



Molecular formula: *Acid* $C_{14}H_{14}F_3N_5O_6S$; *Na salt* $C_{14}H_{13}F_3N_5NaO_6S$
Molecular weight: *Acid* 437.35 g/mole; *Na salt* 459.33 g/mole
Description: White to off-white powder, odorless
Density: 1.63 g/mL (21 C)
Melting point: 170.0 – 177.7 C
Boiling point: NA
Vapor pressure: $<1 \times 10^{-5}$ Pa (25 C)
Stability: Hydrolysis: half-life 20 d (pH 7, 25 C)
Photolysis: half-life 7 h (25 C)
Solubility: Water: 5016 mg/l (pH 7, 25 C)
pK_a: 4.76 (20 C)
K_{ow}: log K_{ow} = -0.43 (pH 7)

HERBICIDAL USE

Trifloxysulfuron sodium is a postemergence herbicide in development for use in cotton and sugarcane. As ENFIELD™ the 75WG can be applied as a broadcast or directed spray, as a single or split application, in conventional or glyphosate tolerant cotton for control of many broadleaf weeds including *Abutilon threophrasti, Acanthospermum hispidum, Amaranthus retroflexus, Senna obtusifolia, Chenopodium album, Ipomoea* spp., *Sesbania exaltata,* and *Xanthium strumarium*. As KRISMAT™ (a premix of trifloxysulfuron sodium plus ametryn) the 75WG can be used on both planted and ratoon cane for season-long control of grass and broadleaf weeds including: *Amaranthus retroflexus, Brachiaria decumbens, Brachiaria plantaginea* Commelina benghalensis, *Euphorbia heterophylla, Ipomoea spp, Rottboellia exaltata,* and *Sorghum halepense (seedling).*

USE PRECAUTIONS

Fire hazard: Not highly flammable, not explosive, no self ignition
Corrosiveness: Not corrosive
Storage stability:
Temperate climates: at least 3 years
Hot climates*:* at least 2 years
Cleaning glassware/spray equipment: Clean spray equipment with 1% v/v household ammonia (3%) concentrate) using sufficient solution to thoroughly rinse all surfaces. See label for detailed cleaning procedures.
Emergency exposure: If poisoning is suspected, stop work immediately and call a physician. Show label to the physician. In case of contact with skin, remove contaminated clothing, wash affected body parts immediately with plenty of water and soap. Rinse splashes from eyes with abundant fresh and clean water for several minutes. If inhaled move to clean air. If swallowed, repeatedly administer medicinal charcoal in plenty of water.
Incompatibilities: See label for up-to-date guidelines.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)
Symptomology: Cessation of growth, chlorosis, death of apical meristems, followed by whole plant death in 1 to 3 weeks. Some weeds, such as *Cassia obtusifolia*, are particularly susceptible to trifloxysulfuron sodium and die a few days after treatment.
Absorption/translocation: Both shoots and roots adsorb trifloxysulfuron and each contributes to its biological activity. Selectivity to cotton is due to differential absorption and metabolism of trifloxysulfuron sodium.
Metabolism in plants: Metabolism via Smile's rearrangement, bridge cleavage, various hydrolytic, oxidative, and conjugation reactions
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: Sulfonylurea resistant weeds have an altered herbicide binding site in the ALS target enzyme.

BEHAVIOR IN SOIL

Sorption: Strongly affected by soil texture and pH
K_{OC}: 29-574 mL/g
Transformation:Photodegradation: Susceptible to indirect photodegradation
Other degradation: Trifloxysulfuron sodium degrades in soil primarily by chemical hydrolysis. This degradation is temperature dependent with a DT_{50} of 52 at 20 C, decreasing to a DT_{50} of 22 at 30 C (each at 75% field capacity). Chemical hydrolysis of trifloxysulfuron sodium in soil is observed over a wide pH range. It is less stable

under acid pH and therefore more rapid degradation may occur in acid soils as compared to alkaline soils. Laboratory studies using water/buffer solutions at 25C show a DT_{50} of 6 d at pH 5, a DT_{50} of 20 d at pH 7 and 21 d at pH 9. Degradation products of trifloxysulfuron sodium in soil have been identified and are not herbicidal.

Persistence: Temperature and moisture contribute significantly to the rapid dissipation (DT_{50}: 5-15 d) of trifloxysulfuron sodium under field conditions. Dry and cool conditions slow down its degradation considerably.

Mobility: Due to the pH dependency of adsorption mobility of trifloxysulfuron sodium ranges from highly mobile to practically immobile in different soils. Under field conditions, trifloxysulfuron sodium is found in the upper layers of the soils and shows little to no tendency to leach.

Volatilization: Due to the low vapor pressure, volatilization is not a significant factor in the dissipation of trifloxysulfuron sodium.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade trifloxysulfuron unless otherwise indicated:

Acute toxicity:

Oral LD_{50} (rat), > 5000 mg/kg; dermal LD_{50} (rat), > 2000 mg/kg; inhalation LD_{50} (rat), > 5.03 mg/L; Non irritant to the skin (93/21 EEC); Non-irritant to the eye (93/21 EEC); Non-sensitizing

Subchronic toxicity: NA

Chronic toxicity: NA

Teratogenicity: Non teratogenic

Reproduction: NA

Mutagenicity: Non mutagenic

Wildlife:

Bobwhite quail oral LD_{50}, > 2000 mg/kg; Mallard Duck oral LD_{50}, > 2000 mg/kg; Daphnia 48-h EC_{50}, > 108 mg/L; Fish 96-h LC_{50}, > 103 mg/L; Eastern Oyster 96-h EC_{50}, > 103 mg/L; Mysid Shrimp 96-h, LC_{50} = 60 mg/L; Earthworm LC_{50}, > 1000 mg/kg soil

Use classification: NA

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: Confidential

Purification of technical: Contact Syngenta Crop Protection

Analytical methods: Contact Syngenta Crop Protection

Historical: U.S. Patent number: 5,403,814.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Syngenta Crop Protection

Reference(s):

1. M. Hudetz, K. Kreuz, A. Steinemann, P. Boutsalis, W. Rueegg, J. Wells, J. E. Soares. 2000. Proc. International Weed Science Congress. 3:124.
2. M. Hudetz, W. Foery, J. Wells, J. E. Soares. 2000. Proc. Southern Weed Science Society. 53:163–166.

trifluralin

CAS #: 1582-09-08

14$^{(E)}$

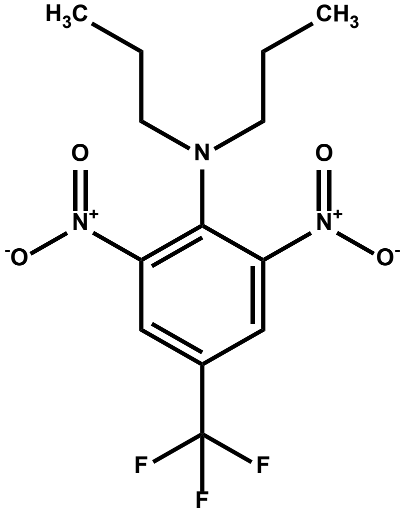
2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl(benzenamine)

NOMENCLATURE

Common name: trifluralin (ANSI, BSI, ISO, JMAF, WSSA)
Other name(s): EL-152; L-36352; trifluraline; 2,6-dinitro-*N*,*N*-dipropyl-4-trifluoromethylaniline; α,α,α-trifluoro-2,6-dinitro-*N*,*N*-dipropyl-p-toluidine (IUPAC)
Trade name(s): ADVANCE®; BAYONET®; BUCKLE®; CLASS®; ELANCOLAN; FLORENE; FREEDOM®; GOWAN TRIFLURALIN; HERITAGE®; PASSPORT®; PRO-MATE® TURF FERTILIZER CONTAINS TEAM PRO 0.86%; SEGURO CARPIDOR; SHOWCASE™; SNAPSHOT® 2.5 TG; SUPER T; TEAM®; TRILLIN®; TRI-4™; TRI-SCEPT®; TREFLAN® 4 EC; TREFLAN® TR-10; TRIFLURALIN; TICHREY®; TRIFLUREX® HFP; TREFANOCIDE; TREFICON; TRIM; QR5® GRANULE
Chemical family: dinitroaniline

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:
trifluralin



Molecular formula: $C_{13}H_{16}F_3N_3O_4$
Molecular weight: 335.28 g/mole
Description: Orange crystalline solid, no appreciable odor
Density: 1.36 g/mL (22 C)
Melting point: 46-47 C
Boiling point: 96-97 C (24 Pa); 139-149 C (560 Pa)
Vapor pressure: 1.47 x 10^{-2} Pa (25 C)
Stability: Decomposed by UV light; decomposes at 275 C
Solubility:
water 0.3 mg/L (25 C)
organic solvents g/100 mL (25 C):
acetone >100   *n*-hexane 5-6.7
acetronitrile >100   methanol 3.3-4
chloroform >100   methyl cellosolve 44
dichloromethane >100
methyl ethyl ketone 88
dimethylformamide 82
toluene >100
dioxane 83
xylene 81
ethyl acetate >100
pK$_a$: None (non-ionizable)
K$_{ow}$: 118,000 (25 C)

HERBICIDAL USE

Trifluralin is labeled for use on more than 80 crops. Primary uses include the following PPI at 0.84-1.12 kg ai/ha water-incorporated (including chemigation) at 2.24 kg ai/ha in established alfalfa; PPI at 1.12-2.24 kg ai/ha in dormant asparagus; PPI at 0.56-1.12 kg ai/ha in drybeans, carrots, castor beans, celery, chicory, endive, transplanted cole crops, okra, peas, peppers, sunflowers, and trees (new plantings); PPI at 0.56-0.84 kg ai/ha in guar, mung beans, lima beans, snap beans, direct-seeded cole crops, greens, mustard, peanuts, canola, crambe, rapeseed, and forage legumes in the Conservation Reserve Program; PPI at 0.84-1.4 kg ai/ha in safflowers; fall PPI, spring PPI, or spring post-plant incorporated at 0.34-0.84 kg ai/ha in spring wheat and barley; PPI or post-plant incorporated at 0.56-1.12 kg ai/ha in winter wheat; fall PPI at 1.12-1.4 kg ai/ha; spring PPI at 0.56-1 kg ai/ha, or via chemigation at 0.84-1.4 kg ai/ha in soybeans; POST incorporated at 0.42-2.24 kg ai/ha or POST using chemigation at 0.84-2.24 kg ai/ha in corn and grain sorghum before weed emergence; fall or spring PPI at 0.84-2.24 kg ai/ha, layby incorporated, or POST via chemigation at 0.84-1.4 kg ai/ha in cotton; directed-POST incorporated at 0.56-1.12 kg ai/ha in cucurbits and tomatoes; directed-POST incorporated in 0.56-1.4 kg ai/ha in onions; fall PPI at 0.56-1.12 kg ia/ha in flax; post-plant incorporated at 0.56-1.12 kg ai/ha or via chemigation at 0.56-0.84 kg ai/ha in potatoes; PPI at 0.56-2.24 kg ai/ha in vines (new plantings); and POST incorporated at 0.56-0.84 kg ai/ha in sugarbeets. Trifluralin also is used on nursery stock, ornamental shrubs, ground covers, established flowers, and under paved surfaces. It should be soil incorporated within 24 hr of application to prevent losses. Trifluralin primarily controls annual grasses, but also controls certain small-seeded broadleaf weeds. In addition to application by conventional sprayer, trifluralin can be impregnated on dry fertilizer or applied in liquid fertilizer and through chemigation systems.

USE PRECAUTIONS

Fire hazard: Trifluralin technical is non-flammable. Flash point of TREFLAN HFP is 99 C (PMCC)
Corrosiveness: Technical is non-corrosive
Storage stability: Shelf life of technical and formulated products is >5 yr.
Cleaning glassware/spray equipment: Clean equipment with detergent and water
Emergency exposure: Flush skin with water. Discomfort

may result from inhalation of EC vapor; consult a physician.

Incompatibilities: Compatible with hard water and other pesticides; compatible with liquid fertilizers although a compatibility adjuvant may be needed

BEHAVIOR IN PLANTS

Mechanism of action: Mitotic disruption through inhibition of the microtubule protein tubulin (more details on page 12)

Symptomology: Most susceptible annual grasses and small-seeded broadleaf weeds fail to emerge, due to inhibition of coleoptile growth or hypocotyl unhooking. Seed germination is not inhibited. Root growth inhibition is a prominent symptom on emerged seedlings and established plants, especially in development of lateral and secondary roots. Roots appear shrubby with tips becoming thickened. Grass stems such as corn may be purple near the base. The base of grass shoots swell, appearing bulbous, and the hypocotyl may swell in broadleaves. Shoots may be deformed and brittle.

Absorption/translocation: Absorbed primarily by emerging plant shoots (grass coleoptile, broadleaf hypocotyl or epicotyl), secondarily by seedling roots. Some absorption of trifluralin vapor may occur. Absorbed trifluralin accumulates at concentrations much higher than in the soil or other external medium. This probably does not represent energy-dependent transport since trifluralin appears to bind tightly to lipid components of cell membranes. In some cases, higher lipid content seeds, roots, or cotyledons has been associated with greater trifluralin tolerance. Plants beyond the seedling stage readily absorb trifluralin into the roots but acropetal translocation to shoots is limited. Trifluralin is highly lipophilic and is rapidly partitioned into membranes and other lipid contents of root tissues, thereby limiting translocation to the shoots (8).

Metabolism in plants: Trifluralin appears to be relatively slowly metabolized in many plants (3, 4), although sweet potatoes and peanuts metabolized 83 and 99%, respectively, after 3 d (2). Identifiable metabolites primarily are derived from one- or two-step *N*-dealkylation, reduction of NO_2 groups to NH_2, and oxidation to produce the phenol derivatives.

Non-herbicidal biological properties: Trifluralin and other dinitroanilines suppress root rot in peas (caused by *Aphanomyces euteiches*) by reducing growth of fungal mycelia and reproduction (11).

Mechanism of resistance in weeds: Trifluralin-resistant goosegrass from the southern U.S. also is resistant to other dinitroaniline herbicides (7). The resistance mechanisms may involve either a change in the binding site on tubulin subunits (13) or an altered microtubule-associated protein (14). Trifluralin-resistant green foxtail has developed in Manitoba, Canada (6). The suggested resistance mechanism is an alteration in an element involved in cytoskeltal function (10). In Australia, a biotype of rigid ryegrass (Lolium rigidum) selected by diclofop use is cross-resistant to trifluralin, chlorsulfuron, and most aryloxyphenoxypropionate and cyclohexanedione herbicides (9). The mechanism is not yet clear but probably involves enhanced rates of herbicide metabolism.

BEHAVIOR IN SOIL

Sorption:

Trifluralin is strongly adsorbed to soil with a Freundlich coefficient, normalized for organic carbon content (K_{OC}), of 6414 to 13414 mL/g (mean 8765 mL/g). This indicates trifluralin as being 'non-mobile' according to most classification schemes.

Transformation:

Photodegradation: Photodegradation of trifluralin on a soil surface under artificial sunlight proceeded with a first-order DT_{50} of 44 days.

Other degradation:

Trifluralin was steadily degraded in soil under aerobic conditions, the rate of degradation was found to correlate well to first-order kinetics. Soil degradation DT_{50}(lab) values ranged between 81 and 356-days at 22°C (mean 181-days), with degradation tending to be fastest in soils with low organic carbon..

Persistence:

European and US field studies showed that trifluralin dissipates slowly in soil, with DT_{50}(field) and DT_{90}(field) values for the EC formulation ranging from 35 375 days (mean 164 days) and 116-1246 days (mean 544 days), respectively. Slower degradation in colder climates is supported by comparing dissipation data between the European and US trials where temperatures in the European trials were generally lower than in the US, and where dissipation was slower. Rates of application and nitrogen fertilization were found to have no noticeable effects on the dissipation of trifluralin, while straw incorporation was observed to increase dissipation. In addition, substitution of ploughing with harrowing during a three year crop rotation, was found not to affect the persistence.

Mobility: Low to negligible leaching potential due to strong absorption to soil

Volatilization: Trifluralin is slightly volatile leading to small but significant losses when left unincorporated on moist soil.

Formulation effects: Granular formulations are less susceptible to losses by volatilization and photodecomposition.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade trifluralin unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat and mouse, >5,000 mg/kg; rabbit and dog, >2000 mg/kg; Dermal LD_{50}, >5000 mg/kg; 4-h inhalation LC_{50}, >4.66 mg/L (20% milled concentrate formulation); Skin irritation rabbit, none; Skin sensitization guinea pig, yes; Eye irritation rabbit, slight.

Subchronic toxicity:

90-d dietary, rat: NOEL <40 mg/kg/d

Chronic toxicity:

24-mo dietary mouse: Systemic NOEL 7.5 mg/kg/d ; No evidence of oncogenicity upto the highest dose tested.

24-mo dietary, Fischer 344 rat: NOEL 40 mg/kg/d (Males) 53 mg/kg/d (Females);. Evidence of oncogenicity at high doses, leading to EPA to classify trifluralin as a Class C carcinogen; in seven other studies with mice and rats, trifluralin showed no signs of oncogenicity.

12-mo dietary, dog: NOEL 2.4 mg/kg/d; reduced body weight gain and slight alerations in clinical pathology at 40 mg/kg/d.

Teratogenicity:

Rat and rabbit: NOEL NA; not teratogenic at up to the highest doses tested (1000 mg/kg/d –rats, 500 mg/kg/d-rabbits)

Reproduction:

Rat: NOEL NA; not a reproductive toxin up to high doses tested 2000 ppm.

Mutagenicity:

Gene mutation: Ames, test, negative; Mouse lymphoma (L5178Y TK$^+$) forward mutation, negative

Structural chromosome aberration: *In vivo* Chinese hamster bone marrow/SCE, negative; CHO, negative; Rat dominant lethal, negative

DNA damage/repair: Rat primarily hepatocytes/ UDS, negative

Wildlife

Bobwhite quail oral LD_{50}, >2000 mg/kg; 8-d dietary LC_{50}, >5000 mg/kg; Mallard duck 8-d dietary LC_{50}, >5000 mg/kg; Fowler's toad 96-h LC_{50}, 0.11 mg/L; Earthworm LC_{50} in soil, >27 mg/kg; Daphnia 48-h LC_{50}, 0.25 mg/L; Bluegill sunfish 96-h LC_{50}, 0.058 mg/L; Channel catfish 96-h LC_{50}, 0.21 mg/L; Fathead minnow 96-h LC_{50}, 0.105 mg/L; Largemouth bass 96-h LC_{50}, 0.075 mg/L; Rainbow trout 96-h LC_{50}, 0.041 mg/L; Sheepshead minnow 48-h LC_{50}, 0.19 mg/L; Bay mussel 96-h LC_{50}, 0.24 mg/L; Grass shrimp 48-h LC_{50}, 0.638 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: Dissolved in hexane and passed over a Florisil column. The first orange-colored band is pure trifluralin. Recrystallize from hexane as necessary.

Analytical methods: Trifluralin concentration in formulated products can be determined as follows: 1) partition into *n*-hexane and measure absorption at 376 nm after removal of colored impurities (5); 2) dissolve or extract the sample in chloroform, then determine by GC using flame ionization detection (12). Residue determination requires extraction of crop tissue or soil with a solvent such as methanol, removal of interfering substances on a Florisil column, and determination by GC with electron affinity detection (12). Test sensitivity is 5-10 mg/kg.

Historical: First described as a chemical by Q. F. Soper in U.S. patent 3,257,190, and as an herbicide in 1960 (1).

MANUFACTURER(S) AND INFORMATION SOURCE(S)

Industry source(s): Adama; Agriliance; Albaugh/Agri Star; BASF; Dow AgroSciences; Drexel; Gowan; Helena; Monsanto; Monterey; UAP-Platte; Setre Chemical; Tenkoz; Wilbur-Ellis

Reference(s):

1. Alder, E. F. et al., 1960. Proc. North Cent. Weed Control Conf. 16:23.
2. Biswas and Hamilton. 1960. Weed Sci. 17:206.
3. Funderburk, H. H. et al. 1967. Proc. South Weed. Conf. p. 39.
4. Golab, T. et al. 1967. J. Agric. Food Chem. 15:638.
5. Holzer, F. J. et al. 1963. J. Assoc. Off. Anal. Chem. 46:659.
6. Morrison, I. N. et al. 1989. Weed Technol. 3:554.
7. Mudge, L. C. et al. 1985. Weed Sci. 32:591.
8. Penner, D. 1971. Weed Sci. 19:571.
9. Powles, S. B. et al. 1990. Pages 394-406. In M.B. Green, H.M. LeBaron, and W.K. Moberg, eds. Managing Resitance to Agrochemicals. Am. Chem. Soc. Symp. Ser. 421, Washington, DC.
10. Smeda, R. J. et al. 1991. Abstr. Weed Sci. Soc. Am. 31:47.
11. Teasdale, J. R. et al. 1979. Weed Sci. 27:195.
12. Tepe and Scoggs. 1967. Pages 527 *in* G. Zweig, ed., Analytical Methods for Pesticides, Plant Growth Regulators and Food Additives, Vol. 5 Academic Press, New York.
13. Vaughn, K. C. et al. 1987. Plant Physiol. 83:956.
14. Vaughn, K. C. et al. 1990. Weed Technol. 4:157.
15. Vaughn and Lehnen. 1991. Weed Sci. 39:450.

triflusulfuron-methyl

CAS #: 126535-15-7 **2$^{(B)}$**

methyl 2-[[[[4-(dimethylamino)-6-(2,2,2-trifluoroethoxy)-1,3,5-triazin-2-yl]amino]carbonyl]amino]sulfonyl]-3-methylbenzoate

NOMENCLATURE

Common name: triflusulfuron (ANSI, ISO, WSSA)

Other name(s): DPX-66037; methyl 2-[4-dimethylamino-6-(2,2,2-trifluoroethoxy)-1,3,5-triazin-2ylcarbamoylsulfamoyl]-*m*-toluate (IUPAC)

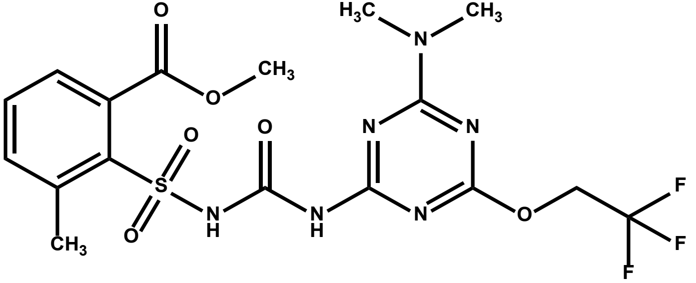
Trade name(s): DEBUT®; SAFARI®; UPBEET®; CARIBOU®

Chemical family: sulfonylurea; triazinylsulfonylurea

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

triflusulfuron-methyl



Molecular formula: $C_{17}H_{19}F_3N_6O_6S$

Molecular weight: 492.43 g/mole

Description: Off-white crystalline solid, vinegar odor

Density: 1.46 g/mL (absolute)

Melting point: 150-154 C

Boiling point: NA

Vapor pressure: 6×10^{-10} Pa (25 C); Henry's Law constant, $<5.8 \times 10^{-10}$ atm m^3/mole (pH 7, 25 C)

Stability: Half-life in water is 3.7 d (pH 5, 25 C); 32 d (pH 7, 25 C); 36 d (pH 9, 25 C); stable in acetonitrile, acetone, methylene chloride, and ethyl acetate; unstable in methanol

Solubility:

water 1 mg/L (pH 3, 25 C); 3 mg/L (pH 5, 25 C); 110 mg/L (pH 7, 25 C); 11,000 mg/L (pH 9, 25 C)

organic solvents g/100 mL (25 C):

acetone 12
acetonitrile 8
chloroform 16
ethyl acetate 2.7
n-hexane 0.00016
methanol 0.7
methylene chloride 58
toluene 0.2.

pK_a: 4.4 (weak acid)

K_{ow}: 9.2 (pH 7, 25 C)

HERBICIDAL USE

Triflusulfuron can be applied early POST in sugarbeets at 17.5-35 g ai/ha for control of broadleaf weeds including bedstraw, kochia, redroot pigweed, shepherdspurse, smartweed spp., velvetleaf, wild mustard, and wild radish.

USE PRECAUTIONS

Fire hazard: Formulated products are non-flammable

Corrosiveness: Formulated products are non-corrosive.

Storage stability: Formulated products do not freeze. Stable during 2 wk at -6 to 54 C

Cleaning glassware/spray equipment: Flush equipment with 1% v/v household ammonia

Emergency exposure: No unusual precautions

Incompatibilities: No physical incompatibilities known. Kochia control may be lower when tank mixed with clopyralid.

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of branched chain amino acid production by inhibition of the enzyme acetolactate synthase (ALS) or acetohydroxy acid synthase (AHAS) (more details on page 12)

Symptomology: Rapid cessation of cell division and plant growth. Plants appear stunted with chlorosis in growing points followed by foliar chlorosis and necrosis.

Absorption/translocation: In young sugarbeets and weeds, <10% of applied is absorbed 20 h after application. Little triflusulfuron is moved out of the leaf when foliar applied.

Metabolism in plants: Selectivity apparently is based on differential rates of metabolism. Half-life of triflusulfuron is 1 h in tolerant sugarbeets, 6-7 h in moderately tolerant weeds such as lambsquarters, and >35 h in susceptible weeds such as *Matricaria* and veronica. Initial metabolism in sugarbeets involves nucleophilic attack by glutathione at the urea carbonyl, producing the *S*-carbamoyl glutathione conjugate plus 7-methylsaccharin and its free acid.

Non-herbicidal biological properties: None known

BEHAVIOR IN SOIL

Sorption: Weakly adsorbed to soil; adsorption decreases as pH increases.

K_{oc} and K_d: K_{oc} 25 mL/g and K_d 0.36 mL/g (sandy loam with 16% clay, 2.5% OM, and pH 7.3); K_{oc} 132 mL/g and K_d 0.5 mL/g (sandy loam with 5% clay, 0.65% OM, and pH 6.2); K_{oc} 47 mL/g and K_d 1.28 mL/g (silty clay with 53% clay, 4.6% OM, and pH 7.4); K_{oc} 52 mL/g and K_d 0.41 mL/g (silt loam with 16% clay, 1.4% OM, and pH 8.2); K_{oc} 35 mL/g and K_d 0.67 mL/g (loamy sand with 5% clay, 3.3% OM, and pH 5.9)

1/n: 0.92-0.94 for adsorption and 0.22-0.47 for desorption

Transformation:

Photodegradation: Half-life on soil is about 13 d for UV-irradiated and non-irradiated samples. Thus, photolysis should be minimal under field conditions. Initial photolysis products are primarily triazine amine and methylsaccharin, with small amounts of triazine urea, *N*-demethylated products, and CO_2.

Other degradation: Primarily degraded in soil by non-microbial hydrolysis of the sulfonylurea bridge to form methylsaccharin and a triazine amine. Methylsaccharin is degraded further by microbes to CO_2 while triazine amine is demethylated relatively rapidly by microbes to *N*-desmethyl triazine amine and *N*,*N*-bis-desmethyl triazine amine; little to no contribution by microbial degradation

Persistence: Triflusulfuron breaks down very rapidly in soil; any rotational crop can be planted 14 d after application.

Field experiments: Degradation half-lives were 2-4 d at the following sites: Madera, California with pH 6.6; Kimberly, Idaho with pH 8.2; Fargo, North Dakota with pH 7.6.

Lab experiments: Degradation followed biphasic kinetics with an initial half-life of 6-14 d. More than 90% of triflusulfuron was degraded within 30 d.

Mobility: Triflusulfuron is mobile, but rapid degradation in soil should prevent leaching under nearly all conditions. No leaching was observed during 18-mo field dissipation studies at three sites. Triflusulfuron is mobile for all of the following: Somersham sandy loam with 2.5% OM, 16% clay, and pH 7.3; Hanford sandy loam with 0.65% OM, 5% clay, and pH 6.2; Fargo-Ryan silty clay with 4.6% OM, 53% clay, and pH 7.4; Portneuf silt loam with 1.4% OM, 16% clay, and pH 8.2; Speyer 2.2 loamy sand with 3.3% OM, 5% clay, and pH 5.9

Volatilization: No loss by volatilization from plant surfaces in the lab

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade triflusulfuron-methyl unless otherwise indicated.

Acute toxicity:

Oral LD_{50} rat, >5000 mg/kg; Dermal LD_{50} rabbit, >2000 mg/kg; 4-h inhalation LC_{50} rat, >5.1 mg/L; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, moderate, clearing in ≤7 d

UPBEET: 4-h inhalation LC_{50} rat, >6.1 mg/L; Skin irritation rabbit, mild; Eye irritation rabbit, moderate, clearing in ≤7 d

Subchronic toxicity:

90-d dietary, mouse: NOEL male 7.13 mg/kg/d, female 166 mg/kg/d

90-d dietary, rat: NOEL male 100 mg/kg; body and liver weight effects

90-d dietary, dog: NOEL 100 mg/kg; hepatotoxic at ≤4000 mg/kg

Chronic toxicity:

18-mo dietary, mouse: NOEL 20.9 mg/kg/d; not oncogenic; liver effects

24-mo dietary, rat: NOEL male 4.06 mg/kg/d, female 750 mg/kg; not oncogenic in females; elevated incidence of benign testicular tumors in males and the NOEL for this lesion was 100 mg/kg

12-mo dietary, dog: NOEL 26.9 mg/kg/d

Teratogenicity:

Rat: NOEL 120 mg/kg/d; maternal and fetal toxicity at ≥350 mg/kg/d; not teratogenic

Rabbit: NOEL dam 15 mg/kg/d, conceptus >800 mg/kg/d; not teratogenic

Reproduction:

Rat: NOEL 5.81 mg/kg/d; body weight effects; not a reproductive toxin

Mutagenicity:

Gene mutation: Ames test, negative; CHO/HGPRT, negative

Structural chromosome aberration: Mouse micronucleus, negative; Unspecified test, positive in 2 of 3 separate trials

DNA damage/repair: UDS, negative

Wildlife:

Bobwhite quail oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Mallard duck oral LD_{50}, >2250 mg/kg; 8-d dietary LC_{50}, >5620 mg/kg; Earthworm LC_{50} in soil, >1000 mg/kg; Honey bee, oral LD_{50}, >1000 mg/kg, topical LD_{50}, >25 µg/bee; Daphnia 48-h LC_{50}, >960 mg/L; Bluegill sunfish 96-h LC_{50}, 760 mg/L; Rainbow trout 96-h LC_{50}, 730 mg/L

UPBEET: Bobwhite quail oral LD_{50}, >2250 mg/kg; Honey bee topical LD_{50}, >25 µg/bee; Daphnia 48-h LC_{50}, >1200 mg/L; Rainbow trout 96-h LC_{50}, 150 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: NA

Purification of technical: NA

Analytical methods: Extraction solvents are acetone:pH 8 $(NH_4)_2CO_3$ buffer (20:80 v/v) for plants and acetonitrile:0.1 M $(NH_4)_2CO_3$ (90:10 v/v) for soil. GC and HPLC methods are available. Successful TLC systems include dichloromethane:methanol:formic acid (95:5:0.2 v/v) and chloroform:acetone:acetic acid:water (60:20:20:0.5 v/v)

Historical: Registration occurred in France and Belgium in 1993.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): DuPont Crop Protection

vernolate

CAS #: 1929-77-7 **$8^{(N)}$**

S-propyl dipropylcarbamothioate

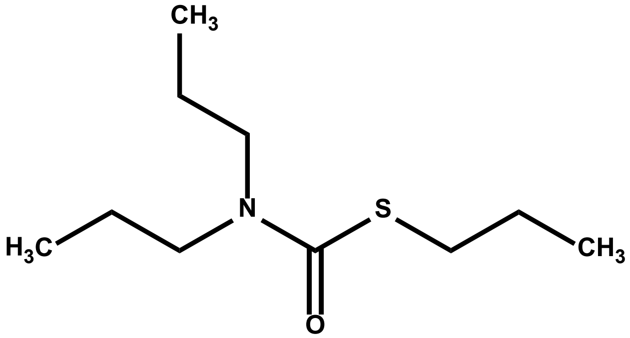
NOMENCLATURE

Common name: vernolate (BSI, ISO, JMAF, WSSA)
Other name(s): R-1607; *S*-propyl dipropyl(thiocarbamate) (IUPAC)
Trade name(s): VERNAM; REWARD; SAVERIT; SAVIROX
Chemical family: carbamothioate; thiocarbamate

CHEMICAL AND PHYSICAL PROPERTIES

Chemical structure:

Vernolate



Molecular formula: $C_{10}H_{21}NOS$
Molecular weight: 203.34 g/mole
Description: Clear, greenish-yellow liquid, sweet and mildly garlic odor
Density: 0.95 g/mL (20 C)
Melting point: NA
Boiling point: 150 C (4.0 x 10^3 Pa)
Vapor pressure: 1.39 Pa (25 C)
Stability: Decomposed by sunlight
Solubility:
 water 108 mg/L (20 C)
 organic solvents:
 miscible in acetone, ethanol, kerosene, methylisobutyl ketone, 4-methylpentan-2-one, xylene
pK_a: None (non-ionizable)
K_{ow}: 6918 (20 C)

HERBICIDAL USE

Vernolate could be applied PPI in soybeans, peanuts, tobacco, and sweet potatoes. Typical rates are 2.2-3.3 kg ai/ha. Vernolate must be incorporated soon after application to prevent volatilization losses. It can be applied in irrigation systems, in liquid fertilizer, or impregnated on dry fertilizer.

USE PRECAUTIONS

Fire hazard: VERNAM 7E is non-flammable; flash point is 121 C (TOC); fire point is 124 C
Corrosiveness: Non-corrosive
Storage stability: Apparently indefinite storage life under normal ambient conditions.
Cleaning glassware/spray equipment: Wash glassware with solvent followed by water; flush equipment with water.
Incompatibilities: None known

BEHAVIOR IN PLANTS

Mechanism of action: Inhibition of fatty acid and lipid biosynthesis (more details on page 13)
Symptomology: Most susceptible grass and broadleaf weeds fail to emerge. Injured dicot crops may have cupped or crinkled leaves with a thick, leathery texture. New leaves are puckered with a “drawstring effect”.
Absorption/translocation: Absorbed by roots and coleoptiles of emerging grass seedlings, although absorption by the coleoptile, especially near the coleoptilar node, is probably most important. Primary absorption in emerging susceptible broadleafs appears to occur in the hypocotyl hook. Vernolate and other thiocarbamates appear to translocate basipetally and acropetally in emerged plants and probably basipetally in emerging seedlings. Translocation likely is unimportant in herbicidal action because vernolate is absorbed very near its site of inhibition.
Metabolism in plants: Vernolate is rapidly metabolized to unidentified metabolites and CO2 in tolerant species such as soybeans and peanuts (1).
Non-herbicidal biological properties: None known
Mechanism of resistance in weeds: No known cases of resistance

BEHAVIOR IN SOIL

Sorption: Vernolate is adsorbed onto dry soil
 K_{oc}: Average is 260 mL/g (5)
Transformation:
 Photodegradation: Vernolate was resistant to photolysis during a 30-d exposure on a thin film of soil.
 Other degradation: Primarily degraded by microbes.
Persistence: Short residual in soil with a typical field half-life of 12 d (5). Vernolate residues do not injure susceptible crops planted 1 yr after application.
 Lab experiments: Half-life in moist loam soil at 21-27 C was ~1.5 wk.
Mobility: Leaching potential is slightly lower than that of EPTC.
Volatilization: Readily lost from a moist soil surface if not incorporated immediately after application.

TOXICOLOGICAL PROPERTIES

Toxicity tests were conducted with technical grade vernolate unless otherwise indicated.

Acute toxicity:
 Oral LD_{50} male rat, 1780 mg/kg, female rat, 1550 mg/kg; Dermal LD_{50} rabbit, 4640 mg/kg; Skin irritation rabbit, none; Skin sensitization guinea pig, no; Eye irritation rabbit, none
 Vernolate 6E: Oral LD_{50} rat ,1800 mg/kg; Dermal LD_{50} rabbit, 10,000 mg/kg

Subchronic toxicity:

90-d dietary, rat: NOEL 32 mg/kg/d

90-d dietary, dog: NOEL >38 mg/kg/d

Chronic toxicity:

18-mo dietary, mouse: NOEL NA; not oncogenic

24-mo dietary, rat: NOEL NA; not oncogenic

12-mo dietary, dog: NOEL NA; not oncogenic

Teratogenicity:

Rat and rabbit: NOEL NA; no fetotoxic or teratogenic effects in the absence of maternal toxicity

Reproduction:

Rat: NOEL NA; not a reproductive toxin

Mutagenicity: Essentially non-genotoxic

Wildlife:

Bobwhite quail 7-d dietary LC_{50}, 12,000 mg/kg; Honey bee oral LD_{50}, 11 μg/bee; Bluegill sunfish 96-h LC_{50}, 8.4 mg/L; Mosquito fish 96-h LC_{50}, 14.5 mg/L; Rainbow trout 96-h LC_{50}, 9.6 mg/L; Three-spined stickleback 96-h LC_{50}, 1-10 mg/L; *Leiostomus xanthurus* 48-h LC_{50}, >1 mg/L

Vernolate 6E: Bobwhite quail 7-d dietary LC_{50}, 14,500 mg/kg; Three-spined stickleback 96-h LC_{50}, 1-10 mg/L

Use classification: General use

SYNTHESIS AND ANALYTICAL METHODS

Synthesis: React *n*-propyl chlorothiolformate with dipropyl amine

Purification of technical: NA

Analytical methods: Vernolate can be separated from impurities on several columns and detected by GC with either thermal conductivity or flame ionization detectors.

Historical: Introduced by Stauffer Chemical Company; U.S. patent 2,913,327.

MANUFACTURER(S) AND INFORMATION SOURCES:

Industry source(s): Drexel Chemical Co.

Reference(s):

1. Ashton, F. M. and A. S. Crafts. 1981. Mode of Action of Herbicides, 2nd ed. John Wiley & Sons, New York.
2. Casida, J. E. et al. 1974. Science 184:573.
3. Fuerst, E. P. 1987. Weed Technol. 1:270.
4. Gronwald, J. W. 1991. Weed Sci. 39:435.
5. Wauchope, R. D. et al. 1992. Rev. Environ. Contam. Toxicol. 123:1.

CHEMICALS PRESENTED IN PREVIOUS EDITIONS

Information on chemicals listed below has been presented in previous editions of the *Herbicide Handbook.* These chemicals have been excluded from this edition. They are no longer in production, use, or development in Canada and the United States, or they are not classified as herbicides or herbicide modifiers. Chemicals are listed by WSSA common name (or by code number, chemical name, or trade name where approved common names are lacking). Presented below are chemical names, trade names, code numbers, manufacturers, and *Herbicide Handbook* editions and page numbers where previously reported, using the following format:

common name
chemical name, eds. (editions) volume no. :page no., volume no. :page no., etc.; if by another chemical name, then ditto; TRADE NAMES by the chemical company; if names by other company or companies, then ditto.

allyl alcohol
propen-1-ol-3, eds. 1:228, 2:297, 3:11, 4:11; 2-propen-1-ol, ed. 4: 11; ALLYL ALCOHOL WEED SEED KILLER by Shell Chemical Co.

arsenic acid
arsenic acid, eds. 1:19, 2:22, *3:25,* 6:15; orthoarsenic acid, eds. 2:22, *3:25,* 4:28, 5:25*;* ZOTOX CRAB GRASS KILLER by Garden Products Co.; DESICCANT L-10 by Pennwalt Corp.

barban
4-chloro-2-butynyl *m*-chlorocarbanilate, eds. 1:51, 2:74, 3:35, 4:37, 5:35; 4-chloro-2-butynyl *N*-(3-chlorophenyl) carbamate, eds. 1:51, 2:74, 3:35, 4:37, 5:35; 4-chloro-2-butynyl 3-chlorophenylcarbamate, ed. 6:20; CARBYNE and CARBYNE 2 by Gulf Oil Corp.; CARBYNE 2 EC and CN-11-1835 by United Agri Products.

benzadox
(benzamidooxy)acetic acid, eds. 3:52, 4:53; TOPCIDE by Gulf Oil Chemical Co.

borate (octa)
disodium octaborate tetrahydrate, eds. 1:155, 2:227, 3:61, 4:62, 5:61, 6:37; POLYBOR by United States Borax & Chemical Corp.; MONOBOR-CHLORATE® by Simplot.

borax
sodium tetraborate, eds. 1:249, 2:316, 3:62, 4:63, 5:63, 6:38; BORASCU, BENZABOR, BOROCTL, DB GRANULAR, NEOBOR, UREABOR, UREABOR 3 1 and UREABOR SD by United States Borax & Chemical Corp.; PYROBOR by Kerr-McGee; BOROCTL™ and UREABOR™ by Simplot.

bulab-37
3,5-dinitro-4-(di-*n*-propylamino)acetophenone, eds. 3 :73, 4:73; BUBAN 37 by Buckman Laboratories Inc.

butam
2,2-dimethyl-*N*-(1-methylethyl)-*N*-(phenylmethyl) propanamide; *N*-benzyl-*N*-isopropyltrimethyl acetamide, ed. 4:78; GCP-5544-6 EC by Gulf Oil Chemical Co.

buthidazole
3-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-4-hydroxy-1-methyl-2-imidazolidinone, eds. 4:480, 5:78; 1-(5-*t*-butyl-1,3,4-thiadiazol-2-yl)-3-methyl-5-hydroxy-1,3-imidazolidin-2-one, eds. 4:480, 5:78; RAVAGE and VEL-5026 by Velsicol.

butralin
4-(1,1-dimethylethyl)-*N*-(1-methylpropyl)-2,6-dinitrobenzenamine, ed. 4:84; AMEX®, MEX® 820, AMCHEM 70-25*,* AMCHEM A-820, TAMEX® by Amchem.

CDAA
2-chloro-*N*,*N*-diallylacetamide, eds. 1 :53, 2: 125, 3:84, 4:92; 2-chloro-*N*,*N*-di-2-propenylacetamide, ed. 5:88; *N*,*N*-diallyl-2-chloroacetamide, eds. 2:125, 3:84, 4:92, 5:88; *N,N*-diallylchloroacetamide, eds. 1:53, 2:125; RANDOX by Monsanto Co.

CDEC (WSSA), sulfallate (BSI, ISO)
2-chloroallyl diethyldithiocarbamate, eds. 1:38, 2:62, 3:87, 4:95; 2-chloroallyl-*N*,*N*-diethyl-dithiocarbamate, ed. 1 :38; VEGADEX by Monsanto Co.

CGA 277476
2-[[[[(4,6-dimethyl-2-pyrimidinyl)amino]carbonyl]amino] sulfonyl]benzoic acid, 3-oxetanyl-ester, Supplement p. 20.; Syngenta.

chloramben
3-amino-2,5-dichlorobenzoic acid, eds. 2:9, 3:90, 4:98, 5:92, 6:51; AMIBEN®, GARDEN WEEDER, ORNAMENTAL WEEDER, VEGIBEN, and WEEDONE GARDEN WEEDER by Amchem Products, Inc.

chlorbromuron
3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea,

eds. 2:38, 3:93, 4:100; MALORAN®, by Ciba-Geigy; BROMEX® by Nor-am.

chlorflurenol
methyl 2-chloro-9-hydroxyfluorene-9-carboxylate eds. 2:263, 3:95, 4: 103, 5:94; 2-chloro-9-hydroxy-9*H*-fluorene-9-carboxylic acid, ed. 6:52. CURBISET and MULTIPROP by Celamerck; MAINTAIN® CF 125 by U.S. Borax.

chloroxuron
N'-[4-(4-chlorophenoxy)phenyl]-*N*,*N*-dimethylurea, eds. 1:66, 2: 104, 6:55; (3-[*p*-(*p*'-chlorophenoxy)phenyl]- 1 , 1 -dimethylurea),ed. 1:66, 2:104, 3:98, 4:106, 5:98; NOREX® by Nor-Am; TENORAN® by CIBA Corp; TENORAN SOW by Ciba-Geigy.

3-CP
2-(*m*-chlorophenoxy)propionic acid, ed. 2:108; 3-CP WETTABLE by Amchem Products, Inc.

cyometrinil
α[(cyanomethoxy)imino]benzene acetonitrile, ed. 5:125; CONCEP® by Ciba-Geigy.

cyprazine
2-chloro-4-cyclopropylamino-6-isopropylamino-1,3,5-triazine, ed. 3:77; 2-chloro-4-(cyclopropylamino)-6-(isopropylamino)-*s*-triazine, eds. 3:113, 4:126; OUTFOX by Gulf Oil Chem. Corp.

dalapon
2,2-dichloropropanoicacid, eds. 1:120, 2:180, 3:123, 4:136, 5:135, 6:80; DOWPON®, DOWPON M, and RADAPON® LIQUID by Dow Chem. Co.; DALAPON® 85 by Fermenta and Diamond Shamrock; REVENGE™ by Hopkins.

diallate
S-(2,3-dichloro-2-propargyl)bis(1-methylethyl) carbamothioate, ed. 7:89; AVADEX by Monsanto.

dichlormate
3,4-dichlorobenzylmethylcarbamate, eds. 1:87, 2:145; SIRMATE and UC 22463 by Union Carbide Corp.

dicryl
3,4-dichloro-2-methacrylanilide, eds. 1:93, 2:149; *N*-(3,4-dichlorophenyl)methaciylamide, eds. 1 :93, 2: 149; DICRYL by FMC Corp. and Niagara Chem. Div.

dimethyldodecylamine acetate
dimethyldodecylamine acetate, ed. 2:208; PENAR by Pennwalt Corp.

dinitramine
N^4,N^4-diethyl-α,α,α-trifluoro-3,5-dinitrotoluene-2,4-diamine, eds. 3:150, 4:169, 5:183. *N*,N^3-diethyl 2,4-dinitro-6-trifluoromethyl- 1 ,3-benzenediamine, eds. 4: 169, 5: 1 83; N^3,N^3-diethyl 2,4-dinitro-6-trifluoromethyl-m-phenylenediamine, ed. 3 : 150; N^3,N^3-diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine; COBEX by United States Borax & Chem. Corp.

dinoseb
2-sec-butyl-4,6-dinitrophenol, eds. 2:52, 3:155, 4:173, 5:187; 2-1(1-methylpropyl)-4,6-dinitrophenol, eds. 1 : 1 *5* 1 , 2:52, 3:155, 4:173, 5:187, 6:105; 4,6-dinitro-o-sec-butylphenol, ed. 1:151; BASANTTE™ and BASANTTE FIVE by BASF Aktiengesellschaft; DINITRO WEED KILLER, DOW GENERAL WEED KILLER, DOW SELECTIVE WEED KILLER, PREMERGE® DN-289, and PREMERGE 3 DINITRO AMINE HERBICIDE by Dow Chem. Co.; DYNAMYTE 3 by Drexel; DYANAP 35 by Uniroyal; VERTAC DINITRO WEEK KILLER by Vertac.

diphenamid
N,*N*-dimethyl-2,2-diphenylacetamide, eds. 1:142, 2:203, 3:159, 4: 177, 5: 191, 6: 107; DYMID by Elanco Products Co. and ENIDE by Upjohn Co.

dipropetryn
6-(ethylthio)-*N*,*N*'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine, ed. 6:109; 2,4-bis(isopropylamino)-6-(ethylthio)-*s*-triazine, ed. 3:163; (2-ethylthio-4,6-bis-isopropylamino-*s*-triazine), ed. 3:163; 2-ethylthio-4,6-bis-isopropylamino-*s*-triazine, eds. 4:181, 5:195; SANCAP 80W by Ciba-Geigy.

DMPA
O-(2,4-dichlorophenyl)*O*-methyl isopropyiphosphoramidothioate, eds. 1:111, 2:171; ZYTRON by Dow Chem. Co.

EL-112 (dithiuron)
N-5-(2-chloro-1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl-*N*,*N'*-dimethylurea, ed. 4:193; Elanco.

erbon
2-(2,4,5-trichlorophenoxy)ethyl 2,2-dichloropropionate, eds. 1:276, 2:344, 3:182; BARON, ERBON R, ERBON 4 by Dow Chem. Co.

ethephon
(2-chloroethyl)phosphonic acid, eds. 2:95, 3:184, 4:204, 5:218, 6:124; CERONE, ETHREL, FLOREL, and PREP by Rhône Poulenc Ag Company; BROMOFLOR, ETHREL, and FLOREL by Amchem Products, Inc. and Union Carbide.

ethiolate
S-ethyl diethylthiocarbamate, ed. 3:186; PREFOX by Gulf Oils Chem. Co.

fenac
2,3,6-trichlorobenzeneacetic acid, eds. 1 :279, 6: 127; (2,3,6-trichlorophenyl)acetic acid, eds. 2:350, 3 : 190, 4:206, 5:224; FENAC, FENAC PLUS, FENAVAR, FENAVAR GRANULAR, FENAMINE, and RACK by Amchem Products, Inc.; TRI-FENE by Tenneco Chemicals, Inc.; FENATROL, FENATROL INDUSTRIAL, FENATROL PLUS, FENAVAR, FENAVAR GRANULAR,

and FENAMINE by Union Carbide; FENATROL® by Rhône-Poulenc Ag. Co.

fenuron
1,1-dimethyl-3-phenylurea, ed. 2:210; 3-phenyl-1,1-dimethylurea, ed. 1:220; *N*,*N*-dimethyl-*N*-phenylurea, ed. 1:220; DYBAR by Du Pont.

fenuron TCA
1,1-dimethyl-3-phenylurea mono (trichloroacetate), eds. 2:2 12, 3:192, 4:209, 5:226, 6:130; 3-phenyl-1,1-dimethylurea trichloroacetate, ed. 1:223; URAB by Allied Chem. Corp.; DOZER by Hopkins.

flamprop-methyl
methyl *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-2-aminopropionate, ed. 5:229; **flamprop:** *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-*DL*-alanine, ed. 5:229]; MATAVEN by Shell Inter. Chem. Co./U.K.

fluchloralin
N-(2-chlorethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl) analine, ed. 4:211. 5:235; *N*-(2-chlorethyl)-2,6-dinitro-N-propyl-4-(trifluoromethyl)benzenamine, ed. 6:134; [*N*-(2-chloroethyl)-α,α,α-trifluoro-2,6-dinitro-*N*-propyl-*p*-toluidine], eds. 4:211, 5:235; BASALIN® by BASF.

fluorodifen
p-nitrophenyl α,α,α-trifluoro-2-nitro-*p*-tolyl ether, eds. 2:286, 3:196; *p*-nitrophenyl 2-nitro-4-(trifluoromethyl) phenyl ether, ed. 2:286; PREFORAN® by Ciba-Geigy; SOYEX® by Nor-AM.

flurenol
n-butyl-9-hydroxyfluorene-(9)-carboxylate, eds. 1 :35, 2:59, 3:198, 4:218, 5:244; [**flurenol-*n*-butyl ester** = 9-hydroxy-fluorene-(9)-carboxylic acid], eds. 1:35, 2:59, 3:198, 4:218; ANITEN, IT 3233 by E. Merck AG; ANITEN, ANITOP, IT 3233 by Celamerck.

glyphosine
N,*N*-bis(phosphonomethyl)glycine, eds. 3:204, 4:228, 5:263; POLARIS® by Monsanto Co.**HCA**
1,1,1,3,3,3-hexachloro-2-propanone, ed. 2:245; hexachloroacetone, ed. 1:170; HCA WEED KTLLER CONCENTRATE by Allied Chem. Corp.

hexaflurate
potassium hexafluoroarsenate, eds. 2:295, 3:210, 4:234, 5:266; NOPALMATE by Pennwalt Corp.

isouron
N'-[5-(1,1-dimethylethyl)-3-isooxazolyl]-*N*,*N*-dimethylurea, ed. 5:280; CONSERVE™ by Elanco.

JV 485
5-[4-bromo-1-methyl-5-(trifluoromethyl)-1*H*-pyrazol-3-yl]-2-chloro-4-fluoro-benzoic acid isopropyl ester; Supplement p 40.

karbutilate
tert-butylcarbamic acid ester with 3-(*m*-hydroxyphenyl)1,1-dimethylurea, eds. 3:220, 4:243, 5:283; *m-(3,3-*dimethylureido)phenyl-tert-butylcarbamate, eds. 3:220, 4:243, 5:283; TANDEX® by FMC and Ciba-Geigy.

MAA
methylarsonicacid, eds. 1:188, 2:260, 3:225, 4:252, 5:289, 6:169; presented as MSMA and DSMA in the 7th edition.

MBR-6033
N-[3-[1,1,1-trifluoromethylsulfony)amino]-4-methylphenyl]acetamide, ed. 3:228; SUSTAR by 3M Co.

metobromuron
3-(*p*-bromophenyl)-1-methoxy-1-methylurea, ed. 2:40; 3(bromophenyl)-methoxy-1-methylurea, ed. 1:30; PATORAN by CIBA Corp.

MON-8000
sodium *N*-(phosphonomethyl)glycine, ed. 5:327; POLADO™ by Monsanto.

monuron
3-(*p*-chlorophenyl)-1,1-dimethylurea, eds. 1:69, 2:110, 3:255; *N*'-(4-chlorophenyl)-*N*,*N*-dimethylurea, eds. 1:69, 2:110, 3:255; TELVAR® and TELVAR ML by Du Pont.

monuron TCA
3-(*p*-chlorophenyl)-1,1-dimethylurea mono(trichloroacetate), eds. 1:74, 2:115, 3:260, 4:289, 5:330; UROX by Allied Chem. Corp.; UROX by Hopkins.

NAA
1-naphthaleneacetic acid, eds. 2:279, 3:262, 4:291, 5:332; AMIDTHIN W, ROOTONE, FRUITONE N, NAA 800, TRANSPLANTONE, and TREHOLD by Amchem Products, Inc. and Union Carbide.

naphthalic anhydride
1,8-naphthalic anhydride, eds. 3:264, 4:293, 5:335; PROTECT by Gulf Oils Chem. Co.

NIA 21844
6-tert-butyl-3-isopropylisoxazolo-[5,4-*d*]pyrmmidin4(5*H*)-one, eds. 3:273, 4:302; FMC.

nitralin
4-(methylsulfonyl)-2,6-dinitro-*N*,*N*-dipropylaniline, eds. 2:274, 3:274, 4:303; PLANAVIN®, PLANAVIN 4 WDL, and PLANAVE 75 WP by Shell Chem. Co.

nitrofen
2,4-dichlorophenylp-nitrophenyl ether, eds. 2:174, 3:278, 4:307, 5:343; 2,4-dichlorophenyl 4-nitrophenyl ether, ed. 1:115; TOK® E-25 and TOK WP-50 by Rohm and Haas.

norea
N,*N*-dimethyl-*N*'-(octahydro-4,7-methano-1*H*-inden-5-yl) urea 3aα,4α,5α,7α,7aα-isomer, ed. 6:194; 3-(hexahydro-

4,7-methanoindan-5-yl)-1,1-dimethylurea, eds. 1:172, 2:274, 3:280, 4:309, 5:345; HERCULES 7351 and HERBAN by Hercules, Inc.; HERBAN by Bristol and by BFC Chemicals.

OCS-21693
methyl 2,3,5,6-tetrachloro-*N*-methoxy-*N*-methylterephthalamate, eds. 1:209, 2:278; Velsicol.

OCS-21799
2-[(4-chloro-o-tolyl)oxy]-*N*-methoxyacetamide, eds. 1:76, 2:12 1; Velsicol.

OCS-21944
O,*S*-dimethyl tetrachlorothioterephthalate, eds. 1:150, 2:218; GLENBAR by Velsicol.

PCP
pentachlorophenol, eds. 1:216, 2:291; DOWICIDE 7 by Dow Chem. Co.; PENTA GENERAL WEED KILLER by Chipman Chem. Co.; SANTOBRITE by Monsanto.

perfluidone
1,1,1-trifluoro-*N*-[2-methyl-4-(phenylsulfonyl)phen-yl] methanesulfonamide, eds. 3:230, 4:325, 5:373; DESTUN® by 3M Co.

potassium azide
potassium azide, eds. 3:306, 4:346; KAZOE by PPG Industries Inc.**PPG-124 (mephenate)**
p-chlorophenyl *N*-methylcarbamate, eds. 3:31 1, 4:351, 5:382; FURLOE 124, PPG-116, PPG-136, PPG-115 and PPG-135 by PPG Industries.

profluralin
N-(cyclopropylmethyl)-α,α,α-trifluoro-2,6-dinitro-*N*-propyl-*p*-toluidine, eds. 3:315, 4:358, 5:386; TOLBAN™ and TOLBAN 4E by Ciba-Geigy Corp.

propazine
6-chloro-*N*,*N*'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine, ed. 6:222; 2-chloro-4,6-bis(isopropylammo)-*s*-triazine, eds. 1:47, 2:70, 3:336, 4:378, 5:410; (2-chloro-4,6-bisisopropylammno-1,3,5-triazine), ed. 1:47; MILOGARD® 80W and PROPAZINE 80W by Geigy Ag. Chemicals; MILOGARD 4L, MILOGARD Maax™, and MTLOCEP® 5L by Ciba-Geigy.

propham
1-methylethyl phenylcarbamate, ed. 6:224; isopropyl carbanilate, eds. 2:251, 3:34 1, 4:382, 5:413; isopropyl *N*-phenylcarbamate, ed. 1:182; CHEM HOE by Chevron, Pittsburgh Plate Glass Co., and by PPG Industries, Inc.

prosulfalin
N-[[4-(dipropylamino)-3,5-dinitrophenyl]sulfonyl]-*S*,*S*-dimethylsulfilimine, ed. 4:388; SWARD by Elanco.

prynachlor
2-chloro-*N*-(1-methyl-2-propynyl)acetanilide, ed. 3:347; BASAMAIZE™ and BAS 2903 H by BASF.

San 6706
4-chloro-5-(dimethylamino)-2-(α,α,α-trifluoro-*m*-tolyl)-3-(211)-pyridazinone, ed. 2:83; San 6706 by Sandoz.

secbumeton
N-ethyl-6-methoxy-*N*'(-1-methylpropyl)-1,3,5-triazine-2,4-di-amine, ed. 4:396; 2-methoxy-4-ethylamino-6-sec-butylamino-*s*-triazine, eds. 2:42 3 :207; 2-sec-butylamino-4-ethylamino-6-methoxy-*s*-triazine, eds. 2:42, 3:207, 4:396; SUMITOL 80W and SUMITOL 3.2 EC by Ciba-Geigy Corp.

sesone
2-(2,4-dichlorophenoxy)ethyl sodium sulfate, ed. 2:159; sodium 2,4-dichlorophenoxyethyl sulfate, ed. 1:245. AMCHEM SESONE by Amchem Products, Inc.

silvex
2-(2,4,5-trichlorophenoxy)propionic acid, eds. 2:347, 3:359, 4:402, 5:429; [2-(2,4,5-trichlorophenoxy)propanoic acid], eds. 4:402, 5:429; WEEDONE 2,4,5-TP by Amchem; KURON® by Dow Chem. Co.; WEEDONE 2,4,5-TP, WEEDONE® CHICKWEED KILLER, and 3D WEEDONE by Amchem and Union Carbide; SILVI-RHAP LV-4TP by Vertac.

sodium arsenite
sodium arsenite, eds. 1:238, 2:307, 3:368: 4:410; ARCADIAN SODIUM ARSENITE "8" SOLUTION by Allied Chem. Corp.; NIAGARA SODIUM ARSENITE WEED KILLER by FMC; KILL ALL SODIUM ARSENITE by Miller Chem. and Fertilizer Corp.; PENITE SODIUM ARSENITE by Pennwalt Corp, Allied Chem. Co., and Rhodia, Inc.

sodium azide
sodium azide, eds. 3:369, 4:412, 5:438; SMITE by PPG Industries, Inc.

SOLAN
3'-chloro-2-methyl-*p*-valerotoluidide; eds. 1:64, 2: 102; *N*-(3-chloro-4-methylphenyl)-2-methylpentanamide, eds. 1:64,2:102; SOLAN by FMC.

SWEP
methyl 3,4-dichlorocarbanilate, ed. 2:269; SWEP by FMC Corp.

2,4,5-T
(2,4,5-trichlorophenoxy)acetic acid, eds. 2:341 , 3:375, 4:418, 5:443; 2,4,5-trichlorophenoxyacetic acid, ed. 1:273; WEEDAR® 2,4,5,-T and WEEDONE® 2,4,5,-T by Amchem and Union Carbide; 2,4,5-T LOW VOLATILE ESTER 6L by Chipman Div. of Rhodia; AMINE 4T, LO-VOL 4T and DECAMINE by Diamond Shamrock; VEON 245 and ESTERON® 245 by Dow Chem. Co.; BRUSH-RHAP A-4T and BRUSHRHAP LV-OXY-4T by Transvaal Inc. and Vertac.

2,3,6-TBA

2,3,6-trichlorobenzoic acid, eds. 1:258, 2:326, 3:378, 4:422; BENZAC 1281 by Amchem; TRYSBEN by Du Pont; FEN-ALL Tenneco; BENZABOR by U.S. Borax; HC-1281 by Heyden.

TCA

trichloroacetic acid, eds. 1:252, 2:319, 3:384, 4:427, 5:447; TCA and DOW SODIUM TCA 90% by Dow Chem. Co.; HOPKINS SODIUM TCA WEED KILLER LIQUID, HOPKINS TCA GRANULAR GRASS WEED KILLER and REVENGE by Hopkins.

TCBC

trichlorobenzyl chloride, eds. 1:267, 2:335, 3:387; RANDOX-T (this formulation contains ca. 1 part CDAA to 2 parts TCBC) by Monsanto Co.

terbutol

2,6-di-tert-butyl-*p*-tolyl methylcarbamate, eds. 1:157, 2:131, 3:397; AZAK, HERCULES 9573 by Hercules, Inc.

terbutryn

N-(1,1-dimethylethyl)-*N*'-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine, ed. 6:244; 2-(tert-butylamino)-4-ethylamino)-6-(methylthio)-*s*-triazine, eds. 2:45, 3:399, 4:436, 5:458; (2-methylthio-4-ethylamino-6-tert-butylamino-*s*-tnazine); eds. 2:45, 3:399; TGRAN® by Ciba-Geigy.

TH 052-H

4,5,7-trichlorobenzthiadiazole-2,1,3, eds. 1:263, 2:331; PH 40-21 by N.Y Philips-Duphar; TH 052-H by Thompson-Hayward.

TIBA

2,3,5-triiodobenzoic acid, eds. 2:357, 3:403; FLORALTONE by Amchem; REGIM 8 by TMC.

tricamba

3,5,6-trichloro-*o*-anisic acid, eds. 1:197, 2:325; 2-methoxy-3,5,6-trichlorobenzoic acid; ed. 1:197; Banvel T (dimethylamine salt), 58-CS-25 by Velsicol.

tritac

2,3,6-trichlorobenzyloxypropanol, eds. 1:270, 2:337; TRITAC, TRITAC-EC, TRITAC-10-G, and TRITAC-D by Hooker Chem. Corp.

UC 20299

sodium *cis*-3-chloracrylate, eds. 1:242, 2:311; PREP and UC 20299 by Union Carbide.

ABBREVIATIONS AND SYMBOLS

A	acre(s)
ae	acid equivalent
ai	active ingredient
ALS	acetolactate synthase
AHAS	acetohydroxyacid synthase
ANSI[1]	American National Standards Institute; prior to 1969 known as American Standards Association (ASA)
ATP	adenosine triphosphate
BSI[1]	British Standards Institute
C	degree(s) Celsius (centigrade)
CAS	Chemical Abstracts Service
CHO	Chinese hamster ovary
cm	centimeter(s)
COC	Cleveland open cup (a method of measuring flammability).
CS	Capsule suspension (formulation): a stable suspension of capsules in a fluid (normally intended for dilution with water before use).
CWSS	Canadian Weed Science Society
d	day(s)
DAT	days after treatment
Dea	diethanolamine
Dma	dimethylamine or dimethylammonium
E	Nomenclature designation from the German word entegen meaning opposite used when higher priority substituent groups of an alkene are on opposite sides of the double bond.
EC	Emulsifiable concentrate: a liquid, homogeneous formulation to be applied as an emulsion after dilution in water.
EC_{50}	Effective concentration: the concentration causing a 50% response in the test system.
ECD	Electron capture detection
EO	Emulsion, water in oil: a fluid, heterogeneous formulation consisting of a dispersion of fine globules of pesticide in water in a continuous organic liquid phase.
EPA	Environmental Protection Agency
EW	Emulsion, oil in water: a fluid, heterogeneous formulation consisting of a dispersion of fine globules of pesticide in an organic liquid in a continuous water phase.
F	degree(s) Fahrenheit
FID	flame ionization detection
FPD	flame photometric detection
g	gram(s)
gal	gallon(s)
GC	gas chromatography
GLC	gas liquid chromatography
GR	Granule (formulation): a free-flowing solid product of a defined granule size range ready for use.
GUS index	Defined as log(half-life) x (4 - log(K_{oc})). The GUS index correlates with pesticide leaching potential. Values of >2.8 indicate high leaching/runoff potential and values of <1.8 indicate low leaching/runoff potential.
h	hour(s)
ha	hectare(s)
HGPRT	hypoxanthine guanine phosphoribosyl transferase
HPLC	high pressure liquid chromatography or high performance liquid chromatography
IAA	indoleacetic acid; auxin
ISO[2]	International Organization for Standardization, Organisation Intemationale de Normalisation
id	inside diameter
inhal	inhalation
IR	infrared
irrit	irritation
IUPAC	International Union of Pure and Applied Chemistry
JAOAC	Journal of the Association of Official Analytical Chemists
JMAF	Japanese Ministry for Agriculture, Forestry and Fisheries
K_d	Soil sorption coefficient: the ratio of sorbed pesticide to dissolved pesticide at equilibrium in a water/soil mixture.
K_f	Adsorption data for herbicides in soil can be expressed by the Freundlich isotherm, $x/m = K_fC^{1/n}$, where x/m is the amount (grams or moles) of herbicide (x) sorbed per weight of dry soil(m), C is the concentration of the herbicide in soil solution at equilibrium, and K_f and 1/n are empirical constants. K_f indicates the amount or extent of herbicide sorption and 1/n is the slope of the $\log_{10}$ of the equation (sorption isotherm) indicating the concentration dependence of K_f and shedding light on the adsorption mechanism. $K_d = K_f$ when 1/n = 1.
kg	kilogram(s)
K_{oc}	Soil organic carbon sorption coefficient: calculated as K_d divided by the weight fraction of organic carbon present in the soil.
K_{ow}	Distribution coefficient between octanol (octan-1-ol) and water
kPa	kilopascal(s)
L	liter(s)
lb	pound(s)
LC	liquid chromatography
LC_{50}	Median lethal concentration: the concentration that kills 50% of the test population.
LD_{50}	Median lethal dose: the dose that kills 50% of the test population.
LOD	Limit of detection
LOAEL	Lowest adverse effect level: the lowest dose at which any adverse effect was observed.
LOEL	Lowest effect level: the lowest dose at which any effect was observed.
LOQ	Limit of quantitation or quantification
M	Molar (moles/L)
m	meter(s)
m	meta
MAC	minimum adverse concentration
MATC	maximum acceptable toxicant concentration
min	minute(s)
mg	milligram(s)
mL	milliliter(s)
mm	millimeter(s)
mo	month(s)
MPa	megapascal(s)
MS	mass spectrometry
MTD	maximum tolerated dose
1/n	see K_f
NA	not available
NCWSS	North Central Weed Science Society
NEWSS	Northeastern Weed Science Society
nm	nanometer(s)
NMR	nuclear magnetic resonance (spectroscopy)
NOEC	no-effect concentration
NOEL	no observable effect level
NOAEL	no adverse effect level
o	ortho
OM	organic matter
oz	ounce(s)
p	para
Pa	pascal
pH	$-\log_{10}$ of hydrogen ion concentration
pK_1	$-\log_{10}$ of the equilibrium constant for the reaction ML M + L, where ML is a metal-ligand complex
pK_a	$-\log_{,0}$ of the acid dissociation constant
pK_b	$-\log_{,0}$ of the base association constant
POST	postemergence
ppb.	parts per billion by weight
PPI	preplant incorporated
ppm .	parts per million by weight
PRE	preemergence
psi	pounds per square inch (lb/inch^2)
®	registered trademark
R	Stereochemistry designation meaning rectus or right representing a clockwise priority of atoms from highest to lowest attached to a chiral center.
s	second(s)
S	Stereochemistry designation meaning sinister or left representing

	a counterclockwise priority of atoms from highest to lowest attached to a chiral center.
SC	Suspension concentrate (formulation): A stable suspension of active ingredients in a fluid intended for dilution with water before use
SCE	sister chromatid exchange
sensitiz.	sensitization
SG	Soluble granule: a formulation consisting of granules to be applied as a true solution of the active ingredient after dissolving in water but which may contain insoluble inert ingredients.
SL	Soluble concentrate: a liquid, homogeneous formulation to be applied as a true solution of the active ingredient after dilution in water.
SP	Soluble powder: a powder formulation to be applied as a true solution of the active ingredient after solution in water but which may contain insoluble inert ingredients.
SWSS	Southern Weed Science Society
TB	Tablet: Solid formulation in the form of small, flat plates.
TCC	Tag closed cup (a method for measuring flammability).
Tea, tea	triethanolamine
Tipa,	tipatriisopropylamine
TLC	thin layer chromatography
TM	trademark
TOC	Tag open cup
UDS	unscheduled DNA synthesis
U.S.	United States
UV	ultraviolet
v/v	volume/volume
WG	Water dispersible granule: a formulation consisting of granules to be applied after disintegration and dispersion in water.
WHO	World Health Organization
WP	Wettable powder: a powder formulation to be applied as a suspension after dispersion in water.
WSWS	Western Society of Weed Science
WSSA	Weed Science Society of America
wt	weight
w/v	weight/volume
yr	year(s)
Z	Nomenclature designation from the German word zusammen meaning together used when higher priority substituent groups of an alkene are on the same side of the double bond.
α	alpha
β	beta
μ	micro (10^{-6}); micron
>	greater than; more than
<	less than; fewer than
/	per
%	percent

[1] American National Standards Institute, 1430 Broadway, New York, NY 10018.

[2] ISO TC81 Secretariat, British Standards Institute, 2 Park Street, London W1A 2B5, England.

ADJUVANTS

Adjuvant Terminology Guidelines

The Adjuvant Terminology Subcommittee of the Weed Science Society of America (WSSA) has worked to assign common names to adjuvants to avoid confusion and eliminate the need of mentioning trade names in *Weed Science* and other WSSA publications. Lack of standardized terminology inhibits effective communication in science and delays acceptance of results of scientific research. The goal of the subcommittee was to develop a system of standardizing adjuvant chemistry into common name terminology. The use of this terminology can be universally applied across scientific disciplines for more effective communication.

To date, only surfactants have been assigned common names. Other adjuvants, such as the non-phytotoxic oils and oil-surfactant blends, have not been assigned common names because of the complexity of oil specifications. Additionally, most of these products are proprietary and their exact composition is unknown. No attempt has been made to assign names to proprietary mixtures of surfactant, alcohol, and water sold by agricultural cooperatives, local dealers, and industry. The exact composition of many of these is unknown and often changes.

The subcommittee first published its report in March 1975 (Weed Science 23: 162-163). Common names were assigned to groups of surfactants within a chemistry class but not to individual surfactants. This system can be used to classify approximately 90% of the surfactants that are expected to be reported in WSSA publications.

Surfactant chemistry is complicated because many surfactants are mixtures of related materials. For example, in the manufacture of surfactants such as nonoxynol or octoxynol (see attached list for chemistries), the appropriate phenolic compound is reacted with ethylene oxide (EO) to produce a product containing a desired number of moles of EO per mole of phenol; but the typical reaction may yield homologous phenol compounds with EO chains of varying length. Further purification is either unnecessary or uneconomical, so a commercial phenolic adjuvant with 9 moles of EO per mole of phenol may actually be a blend of compounds having an average of 9 moles of EO per mole of phenol. Similarly, in the synthesis of ethoxylated alcohols, it is possible that the resulting product may be a blend of materials varying not only in degree of ethoxylation but also in alcohol chain length. Even though such surfactants may be mixtures of related materials, the Environmental Protection Agency (EPA), the Food and Drug Administration (FDA), and other organizations use single chemical names to describe these materials. The chemical names used by EPA, FDA, and others are often complex. Thus, one of the most urgent needs in adjuvant terminology is developing and adopting standardized common names.

Common names of herbicides used by the WSSA are usually approved by the American National Standards Institute Committee on Common Names for Pest Control Chemicals K62 (ANSI-K62) and by the International Standards Organization (ISO). The WSSA is a member of ANSI-K62 and this committee is a member of ISO which works through foreign countries in an effort to standardize common names for agricultural chemicals worldwide. The Adjuvant Terminology Subcommittee contacted ANSI-K62 soliciting their aid in assigning common names to adjuvants but ANSI-K62 voted not to participate. Thus, WSSA common names for adjuvants are not approved by ANSI. Adoption of these single-word names by the WSSA, however, established a system that other scientific organizations are encouraged to use.

Only two organizations in the United States other than WSSA assign common names to surfactants: the United States Adopted Names Council (USAN) and the Cosmetic, Toiletry, and Fragrance Association, Inc. (CTFA). Common names for surfactants used by these organizations usually contain either numbers or letters as prefixes or suffixes, and thus are generally unacceptable to ANST, ISO, and WSSA. Some WSSA common names for surfactants are similar to those used by USAN or CTFA, but this was not possible when these organizations used two or more words for common names.

To date, WSSA uses the chemical names of surfactants used by EPA and FDA in assigning common names. As a result, common names are assigned only to anionic and nonionic surfactants. The assigning of additional common names is continuing.

An in-depth example of assigning common names to surfactants can be made with the Tween series. All of these surfactants have the common name oxysorbic. The chemistry of oxysorbic is polyoxyethylated sorbitol fatty acid esters. Individual surfactants would be reported in WSSA publications as:

A. Tween 60: oxysorbic (20 POE[1]) (polyoxyethylated sorbitan monostearate).
B. Tween 80: oxysorbic (20 POE) (polyoxyethylated sorbitan monoleate).
C. Tween 81: oxysorbic (5 POE) (polyoxyethylated sorbitan monoleate).
D. Tween 20: oxysorbic (20 POE) [polyoxyethylated sorbitan monoleate (polysorbate 20 POE)].

The number in parentheses behind the common name indicates the number of moles of EO[2] per mole of sorbitol fatty acid esters.

All surfactants within a common name class, other than these within oxysorbic, will have the same common and chemical name. Only the degree of ethoxylation (moles) and!or the inorganic salt derivative ofthe individual surfactants will differ. Thus, for example, Triton N-100, Sterox NJ, and Tgepal CO-610 all have 9 to 10 moles of ethoxylation and would be reported as nonoxynol (9 - 10 POE)[α(*p*-nonylphenyl)-ω-hydroxypoly (oxyethylene)].

The subcommittee expresses its appreciation to the many individuals who contributed to this report, especially to those in more than 15 industrial organizations in the surfactant industry who offered suggestions and advice in developing the list of common names. Appreciation is also expressed to Amchem Products, Inc., Ambler, PA; American Cyanamid Co., Princeton, NJ; Armak Co., Chicago,IL; and the Rohm and Haas Co., Philadelphia, PA for use of their legal departments to check common names for possible conflicts.

Valued guidance and encouragement was given by D. L. Klingman, former Chair of the WSSA Terminology Committee.

Common and Chemical Names of Adjuvants

alaminol
Chemistry: *N,N*-bis(2-(ω-hydroxypoly-oxyethylene)ethyl) alkylamine; the reaction product of 1 mole *N,N*-bis(2-hydroxyethyl) alkylamine and 3-60 moles of ethylene oxide, where the alkyl group (C_8-C_{18}) is derived from coconut, cottonseed, soya, or tallow acids. Class: cationic. Type: Fatty amine ethoxylates. Trade names: Rhodameen RN-730 and Ethomeen T-25.

albenate
Chemistry: alkyl(C_8-C_{24})benzene sulfonic acid and its salts. Class: alkylaryl sulfonate. Type: anionic. Trade names: Nacconol series, Calsoft F-90, DDBSA, Rhodacal DS-10, Rhodacel 2283[3].

alfos
Chemistry: α-alkyl(C_{10}-C_{16})-ω-hydroxypoly (oxyethylene) mixture of dihydrogen phosphate esters; indicate POE[1] content as (X) moles[2]. Class: polyoxyethylene alkyl phosphate ester. Type: anionic. Trade names: Emphos CS-13 1, Rhodafac RD-series.
allinateChemistry: α-lauryl-ω-hydroxypoly(oxyethylene) sulfate; indicate POE[1] content as (X) moles[2]. Class: lauryl polyoxyethylene sulfate salts. Type: anionic. Trade names: Rhodapex N-70, Rhodapex ES.

allinol
Chemistry: α-alkyl(C_{11}-C_{15})ω-hydroxypoly(oxyethylene); indicate POE[1] content as (X) moles[2]. Class: $C_{11}C_{15}$ linear, primary alcohol ethoxylate. Type: non-ionic. Trade names: Neodol 25-3, Alfonic 1014-40, RhodasurfL-4.

diocusate
Chemistry: sodium dioctylsulfosuccinate. Class: dioctyl sodium sulfosuccinate. Type: anionic. Trade names: Triton GR-5, Aerosol OT, Geropon 55-0-75.

dooxynol
Chemistry: α-(*p*-dodecylphenyl)-ω-hydroxypoly (oxyethylene) produced by the condensation of dodecylphenol with ethylene oxide; indicate POE[1] content as (X) moles[2]. Type: non-ionic. Trade names: Igepal RC-series, Tergitol 12-P-9, Sterox D-series.

ligsolate
Chemistry: lignosulfonate, NH_4, Ca, Mg, K, Na, and Zn salts[3]. Class: salts of lignosulfonic acids. Type: anionic. Trade names: Marasperse N-22, Polyfon O.

nofenate
Chemistry: α-(*p*-nonylphenyl)-ω-hydroxypoly(oxyethylene)sulfate, NH_4, Ca, Mg, K, Na, Zn salts[3] the nonyl group is a propylene trimer isomer; indicate POE' content as (X) moles[2]. Class: salts of sulfate ester of nonylphenoxypoly(ethyleneoxy) ethanol. Type: anionic. Trade names: Rhodapex CO series.

nonfoster
Chemistry: α-(*p*-nonylphenyl)-ω-hydroxypoly(oxyethylene); mixture of dihydrogen phosphate and monophosphate esters; indicate POE' content as (X) moles[2]. Class: polyoxyethylene nonylphenol phosphate esters. Type: anionic. Trade names: Rhodafac RE-series.

nonoxynol
Chemistry: α-(*p*-nonylphenyl)-ω-hydroxypoly (oxyethylene) produced by the condensation of nonylphenol with ethylene oxide; indicate POE' content as (X) moles[2]. Class: polyoxyalkylene nonylphenol. Type: nonionic. Trade names: Sterox N-series, Makon 6, Igepal CO-series, Triton N-series, T-DET N-series.

nonpoloxamer
Chemistry: α-(*p*-nonylphenyl)-ω-hydroxypoly(oxypropylene)block polymer with poly(oxyethylene). Class: nonylphenol EO/PO block copolymer. Type: nonionic. Trade names: Soprophor SC/167 and Soprophor 724/P.

octoxynol
Chemistry: α[*p*-1, 1,3,3-tetramethyl butyl phenyl]–ω-hydroxypoly(oxyethylene) produced by the condensation of *p*-(1,1,3,3-tetramethylbutyl)phenol with ethylene oxide; indicate POE[1] content as (X) moles[2]. Class: polyoxyethylene octylphenol. Type: nonionic. Trade names: Igepal CA-series, Triton X-series.

oxycastol
Chemistry: castor oil, polyoxy-ethylated; indicate POE[1] content as (X) moles[2]. Class: ethoxylated castor oil. Type: nonionic. Trade names: Alkamuls EL-719, Alkamuls EL-620, Trylox 5909.

oxysorbic
Chemistry: polyoxyethylated sorbitol fatty acid esters[4] indicate POE[1] content as (X) moles[2]. Class: polyoxyethylated sorbitol fatty acid esters. Type: nonionic.

Trade names: Atlox 1045, Drewmulse POE-STS, Tween series, G-1045, Alkamuls PS-series.

poloxamer
Chemistry: poly(oxypropylene) block polymer with poly(oxyethylene). Class: EO/PO block copolymer. Type: non-ionic. Trade names: ANTAROX series and PLURONIC series.

talloil
Chemistry: tall oil, fatty acids not less than 58 percent, rosin acids not more than 44 percent, unsaponifiables not more than 8 percent. Class: tall oil. Type: anionic. Trade names: Acintol FA-1, Pamak4.

thalestol
Chemistry: polyglyceryl phthalate ester of coconut oil fatty acid. Class: modified phthalic glycerol alkyl resin. Type: non-ionic. Trade names: Triton B-1956.

tristyroxynol
Chemistry: α-[2,4,6-tris[1-(phenyl)ethyl]phenyl]-ω-hydroxypoly(oxyethylene). Class: tristyrylphenol ethoxylates. Type: non-ionic. Trade names: Soprophor BSU and Soprophor 5/25.

[1] POE is polyoxyethylene.

[2] The degree of ethoxylation of all materials containing ethylene oxide should be designated within parentheses following the common name for publication in *WeedScience* and other WSSA publications; e.g., both Triton N-100 and Sterox NJ contain 9-10 moles of ethylene oxide per mole of nonylphenol and would be designated nonoxynol (9-10 POE).

[3] For publication, indicate the exact salt used in manufacture, e.g., calcium lignosulfonate.

[4] For publication, indicate the specific fatty acid used in manufacture of the surfactant, such as monostearate or monoleate, in the chemical name given for the surfactant.

This section originated as a report of the WSSA Adjuvant Terminology Subcommittee composed of C. G McWhorter (chair), W. W. Abramitis, J. R. Bishop, T. N. Jordan, and A. J. Tafuro. The report was published in *Weed Science* 26:204-205. Additional adjuvant names for the *Herbicide Handbook* were submitted by the Adjuvant Terminology Subcommittee, composed of E. P. Richard (chair), G. B. Beestman, J. A. Garr II, J. L. Hazen, K. Khodayari, and G D. Wills.

TERMS AND DEFINITIONS

The following definitions were developed by WSSA committees. They are included here for the convenience of Herbicide Handbook readers and to encourage the use of standardized terminology in WSSA publications. Some terms are defined only in their specific weed science context, while recognizing that other definitions apply for common or general English usage. Soil terms were taken from a December 1, 1978 report ofthe WSSA Soils Terminology Subcommittee including J. Boehle, Jr. (chair), J. Alexander, E. Chamberlain, D. Finnerty, A. Hiltbold, C. Reick, and K. Savage (reviewed by D. E. Smika). Other terms were compiled by the WSSA Terminology Committee including T. R. Harger (chair), P. A. Banks, A. R. Bell, J. H. Dawson, W. R. Mullison, D. T. Patterson, and J. R. Teasdale (with assistance from J. B. Baker, D. E. Davis, L. M. Kitchen, and B. Truelove).

Absorption - The process by which a herbicide passes from one system into another, e.g. , from the soil solution into a plant root cell or from the leaf surface into the leaf cells.

Acid equivalent (ae) - The theoretical yield of parent acid from a pesticide active ingredient which has been formulated as a derivative.

Acid soil - Soil with a pH value <7.0.

Acropetal - Toward the apex of a plant organ; generally upward in shoots and downward in roots. Opposite of basipetal.

Activation - The process by which a surface applied herbicide is moved into the soil where it can be absorbed by emerging seedlings. This is normally accomplished by rainfall, irrigation, or tillage. Activation does not imply any chemical change in the active ingredient.

Active ingredient (ai) - The chemical in a herbicide formulation primarily responsible for its phytotoxicity and which is identified as the active ingredient on the product label.

Acute toxicity - The quality or potential of a substance to cause injury or illness shortly after exposure. See chronic toxicity.

Adjuvant - Any substance in an herbicide formulation or added to the spray tank to modify herbicidal activity or application characteristics.

Adsorption - The process by which an herbicide associates with a surface, e.g., a soil colloidal surface.

Agroecosystem - An ecosystem managed for crop production.

Alkaline soil - Soil with a pH >7.0.

Allelopathy - The adverse effect on the growth of plants or microorganisms caused by the action of chemicals produced by other living or decaying plants.

Anion exchange capacity - The sum total of exchangeable anions that a soil can adsorb. Expressed as moles or mmoles of positive charge per kg of soil (or other exchange material).

Apoplast - The total, non-living continuum in a plant, including cell walls, intercellular spaces, and the xylem vessels, that forms a continuous permeable system through which water and solutes may move.

Antagonism - An interaction of two or more chemicals such that the effect when combined is less than the predicted effect based on the activity of each chemical applied separately.

Antidote - (1) A chemical applied to prevent the phytotoxic effect of a specific herbicide on desirable plants (Synonymous with protectant). (2) A substance used as a medical treatment to counteract herbicide poisoning.

Available nutrient - That quantity of a nutrient element or compound in the soil that can be readily absorbed and assimilated by growing plants.

Available water - The portion of water in a soil that can be absorbed by plant roots; considered by most workers as the amount of water released by the soil when the equilibrium soil water matrix potential is decreased from field capacity to 1500 joules/kg.

Band treatment - Applied to a linear restricted strip on or along crop rows rather than continuous over the field area.

Basal treatment - Applied to encircle the stem of a plant just above the soil surface such that foliage contact is minimal. A term used mostly to describe treatment of woody plants.

Base-saturation percentage - The extent to which the adsorption complex of a soil is saturated with exchangeable cations other than hydrogen. It is expressed as a percentage of the total cation exchange capacity.

Basipetal - Toward the base of a plant organ; generally downward in shoots and upward in roots. Opposite of acropetal.

Bed - (1) A ridge or elevated strip of soil formed for planting crops above furrows on each side. (2) An area in which seedlings or nursery stock are grown for later transplanting in the field.

Bioassay - Quantitative or qualitative determination of herbicide by use of sensitive indicator plants or other biological organ-isms.

Biological control of weeds - Control or suppression of weeds by the action of one or more organisms, through natural means, or by manipulation of the weed, organism, or environment.

Biotic interference - The adverse effect of one organism or population in a common ecosystem on another by attracting, encouraging, or harboring one or more intermediate organisms.

Biotype - A population within a species that has a distinct genetic variation.

Blind cultivation - Cultivation before seeded crops emerge.

Boot or Booting - A growth stage of grasses (including cereal crops) when the upper leaf sheath swells due to the growth of the developing spike or panicle.

Broadcast rate equivalent - For band treatments, it is the amount of herbicide applied per unit area when only the band area is considered. All rates for band treatment should be expressed as the broadcast rate equivalent.**Broadcast treatment -** Applied as a continuous sheet over the entire field.

Brush control - Control of woody plants such as brambles, sprout, clumps, shrubs, trees, and vines.

Calcareous soil - Soil containing sufficient free calcium carbonate or calcium-magnesium carbonate to effervesce visibly when treated with cold 0.1 M HCl in water.

Caliche - A layer near the surface, more or less cemented by secondary carbonates of Ca or Mg precipitated from the soil solution. It may occur as a soft thin soil horizon, as a hard thick bed beneath the solum, or as a surface layer exposed by erosion.

Carcinogenic - Capable of causing cancer in animals.

Carrier - A gas, liquid, or solid substance used to dilute or suspend a herbicide during its application.

Cation exchange capacity (CEC) - The sum total of exchangeable cations that a soil can adsorb. Expressed as moles or mmoles of negative charge per kg of soil (or of other exchange material).

Chemical name - The systematic Name of a chemical compound according to the rules of nomenclature of the International Union of Pure and Applied Chemistry (IUPAC), Chemical Abstracts Service, or other organization. Chemical names presented in this handbook are those of the Chemical Abstracts Service.

Chemotype - A group of organisms that produce the same profile for a particular class of chemicals such as chalcones, aurones, flavanols, etc.

Chiorosis - Loss of green color (chlorophyll) from foliage.

Chronic toxicity - The quality or potential of a substance to cause injury or illness after repeated exposure over an extended perod of time.

Clay - (1) A soil separate consisting of particles <0.002 mm in equivalent diameter (2) A soil textural class; soil containing 40% or more clay, <45% sand, and <40% silt.

Clay loam - A soil textural class; soil containing 27-40% clay and 20-45% sand.

Clod - A compact, coherent mass of soil ranging in size from 5-10 mm to as much as 20 or 25 cm; produced artificially, usually by the activity of man by tillage, digging, etc., especially when these operations are performed on soils that are either too wet or too dry for normal tillage operations.

Coarse-textured soil - The texture exhibited by sands, loamy sands, and sandy loams except very fine sandy loam.

Common name - A generic name for a chemical compound.

Community - The populations of species living in a common ecosystem.

Compatibility - The characteristic of a substance, especially a pesticide, of being mixable in a formulation or in the spray tank for application in the same carrier without undesirably altering the characteristics or effects of the individual components.

Competition - The active acquisition of limited resources by an organism which results in a reduced supply and consequently reduced growth of other organisms in a common environment.**Concentration -** For herbicides, the quantity of active ingredient or parent compound equivalent expressed as moles or mass per unit volume or per unit mass of the resulting solution or mixture. Expressions of percent should be avoided or used only for expressions of mass per mass.

Contact applicator – A device that applies a herbicide to plants by direct contact of the applicator and the plant.

Contact herbicide - An herbicide that causes injury to only the plant tissue to which it is applied, or a herbicide that is not appreciably translocated within plants.

Cracking - The time just prior to seedling emergence when the soil cracks and the surface is pushed upward by growth of the emerging seedling.

Crust - A surface layer on soils, ranging in thickness from a few millimeters to perhaps as much as 3 cm, that is much more compact, hard, and brittle when dry, than the material immediately beneath it.

Defoliant - A chemical that causes the leaves to abscise from a plant.

Desiccant - Any substance or mixture of substances used to accelerate the drying of plant tissue.

Dicot - Abbreviated term for dicotyledon; preferred in scientific literature over broadleaf to describe plants.

Dicotyledon (dicot) - A member of the Dicotyledoneae; one of two classes of angiosperms usually characterized by the following: two seed leaves (cotyledons), leaves with net venation, and root systems with tap roots.

Diluent - Any gas, liquid, or solid material used to reduce the concentration of an active ingredient in a formulation.

Directed application - Precise application to a specific area or plant organ such as to a row or bed or to the leaves or stems of plants.

Dispersible granule - A dry granular formulation that will separate or disperse to form a suspension when added to water.

Dormancy - The state of inhibited seed germination or growth of a plant organ when in an environment normally conducive to growth.

Dust mulch - A loose, finely granular, or powdery condition on the surface of the soil, usually produced by shallow cultivation.

Ecosystem - An ecological entity consisting of the biotic community and the non-living environment functioning together in an inseparable interacting system.

Ecotype - A population within a species that has developed a distinct morphological or physiological characteristic (e.g., herbicide resistance) in response to a specific environment and that persists when individuals are moved to a different environment.

Edaphic - (1) Of or pertaining to the soil. (2) Resulting from or influenced by factors inherent in the soil or other substrate, rather than by climatic factors.

Emergence - The event in seedling establishment when a shoot becomes visible by pushing through the soil surface.

Emersed plant - A rooted or anchored aquatic plant adapted to grow with most of its leaf-stem tissue above the water surface and not lowering or rising with the water level.

Emulsifiable concentrate (EC) - A single phase liquid formula-tion that forms an emulsion when added to water. See Abbreviations and Symbols section for the official GIFAP definition used elsewhere in this handbook.

Emulsifier - A substance that promotes the suspension of one liquid in another.

Emulsion - One liquid suspended as minute globules in another liquid (e.g., oil dispersed in water).

Encapsulated formulation - Herbicide enclosed in capsules (or beads) of material to control the rate of release of active ingredient and thereby extend the period of activity.

Environment - The sum total of all biological and physical factors affecting an organism, population, or community.

Epinasty - That state in which more rapid growth on the upper side of a plant organ or part (especially leaf) causes it to bend or curl downward.

Exchange capacity - The total ionic charge of the adsorption complex active in the adsorption of ions. See **Anion exchange capacity** and **Cation exchange capacity.**

Extender - A chemical that increases the longevity of a herbicide in soil.

Fertilizer - Any organic or inorganic material of natural or synthetic origin that is added to a soil to supply one or more elements essential to the growth of plants.

Field capacity - The percentage (expressed on the basis of weight or volume) of water remaining in a soil 2 or 3 d after having been saturated and after free drainage has practically ceased.

Fine-textured soil - Consisting of or containing large quantities of the fine fractions, particularly of silt and clay. Includes clay loam, sandy clay loam, silty clay loam, sandy clay, silty clay, and clay textural classes. Sometimes subdivided into clayey texture and moderately fine texture. See **Soil texture.**

Floating plant - A free-floating or anchored aquatic plant adapted to grow with most of its vegetative tissue at or above the water surface and lowering or rising with the water level.

Flowable - A two-phase formulation containing solid herbicide suspended in liquid and that forms a suspension when added to water.

Formulation - (1) A pesticide preparation supplied by a manufacturer for practical use. (2) The process, carried out by manufacturers, of preparing pesticides for practical use.

Frill treatment - Placement of a herbicide into a series of overlap-ping ax cuts made through the bark in a ring around the trunk of a tree.

Genotype - The entire genetic constitution or set of genes possessed by an organism.

Germination - The process of initiating growth in seeds.

Granular - A dry formulation consisting of discrete particles generally <10 mm^3 and designed to be applied without a liquid carrier. See Abbreviations and Symbols section for the official GIFAP definition used elsewhere in this handbook.

Green manure - Plant material incorporated into the soil while green, or soon after maturity, for improving the soil.

Habitat - The physical location or type of environment in which an organism is normally found.

Hardpan – A hardened soil layer, in the lower A or in the B horizon, caused by cementation of soil particles with organic matter or with materials such as silica, sesquioxides, or calcium carbon-ate. The hardness does not change appreciably with changes in moisture content and pieces of the hard layer do not slake in water.

Head or Heading - A growth stage of grasses (including cereal crops) when the spike or panicle is emerging or has emerged from the sheath.

Herbaceous plant - A vascular plant that does not develop persistent woody tissue above ground.

Herbicide - A chemical substance or cultured biological organism used to kill or suppress the growth of plants.

Herbicide modifier - A chemical substance used with herbicides to change their herbicidal properties by a physiological mechanism. They include safeners, synergists, extenders, etc., but do not include compounds such as surfactants that may modify herbicidal activity by chemical or physical mechanisms.

Herbicide resistance - The trait or quality of a population of plants within a species or plant cells in tissue culture of having a tolerance for a particular herbicide that is substantially greater than the average for the species and that has developed because of selection for naturally occurring tolerance by exposure to the herbicide through several reproductive cycles.

Humus - (1) That more or less stable fraction of the soil organic matter remaining after the major portion of added plant and animal residues have decomposed. Usually it is dark colored. (2) Includes the F and H layers in undisturbed forest soils. See **Soil organic matter.**

Incorporate - To mix or blend a herbicide into the soil.

Interference - For plants; the total adverse effect that plants exert on each other when growing in a common ecosystem. The term includes competition, allelopathy, biotic interference, and other detrimental modifications in the community or environment.

Invert emulsion - The suspension of minute water droplets in a continuous oil phase.

Joint or Jointing - A growth stage of grasses (including cereal crops) when stem internodes begin elongating.

Label - The directions for using a pesticide approved as a result of the registration process.

Lateral movement - Movement of a herbicide through soil, generally in a horizontal plane, from the original site of application.

Layby application - Applied and incorporated with or applied after the last cultivation of a crop.

LC_{50} - The concentration of a substance in air (inhalation toxicity), water (aquatic toxicity) or continual exposure in the diet that will kill 50% of the organisms in a specific test situation.

LD_{50} - The dose (quantity) of a substance that will be lethal to 50% of the organisms in a specific test situation. It is expressed in weight of the chemical (mg) per unit of body weight (kg) and the toxicant may be fed (oral LD_{50}), applied to the skin (dermal LD_{50}), or administered in the form of vapors (inhalation LD_{50}).

Leaching - (1) The removal of materials in solution from the soil. (2) The downward movement of material(s) into a soil profile with soil water (material may or may not be in true solution and may or may not move from soil).

Lime, agricultural - A soil amendment consisting principally of calcium carbonate, but including magnesium carbonate and per-haps other materials used to neutralize soil acidity and furnish calcium and magnesium for the growth of plants.

Loam - A soil textural class; soil containing 7-27% clay, 28-50% silt, and <52% sand.

Loamy sand - A soil textural class; soil containing no more than 85-90% sand, and the percentage of silt plus 1.5 times the percentage of clay is not less than 15%; also, it contains not less than 70-85% sand, and the percentage of silt plus twice the percentage of clay does not exceed 30%.

Loamy soil - Intermediate in texture and properties between fine- and coarse-textured soils. Includes all textural classes with the words ‘loam’ or ‘loamy’ as a part of the class name, such as clay loam or loamy sand. See **Soil texture.**

Macronutrient - A chemical element necessary in relatively large amounts (usually greater than 500 ppm in the plant) for the growth of plants. These elements consist of C, H, 0, Ca, Mg, K, P, 5, and N.

Medium-textured soil - Intermediate between a fine- and coarse-textured soil. Includes very fine sandy loam, loam, silt loam, and silt textural classes.

Metabolite - A compound derived from metabolic transformation of an herbicide by plants or other organisms.

Micronutrient - A chemical element necessary only in extremely small amounts (usually <50 ppm in the plant) for the growth of plants. These elements consist of B, Cl, Cu, Fe, Mn, Mo, and Zn.

Mineral soil - A soil consisting predominantly of, and having its properties determined predominantly by, mineral matter. Usually contains <20% organic matter, but may contain an organic surface layer up to 30 cm thick.

Moisture tension (or pressure) - The equivalent negative pressure in the soil water. It is equal to the equivalent pressure that must be applied to the soil water to bring it to hydraulic equilibrium, through a porous permeable wall or membrane, with a pool of water of the same composition.

Monocot - Abbreviated term for monocotyledon; preferred in scientific literature over grass to describe plants.

Monocotyledon (monocot) - A member of Monocotyledoneae; one of two classes of angiosperms, usually characterized by the following: one seed leaf (cotyledon), leaves with parallel venation, root systems arising adventitiously and usually diffuse (fibrous).

Muck soil - (1) A soil containing between 20 and 50% of organic matter. (2) An organic soil in which the organic matter is well decomposed (USA usage).

Mulch - (1) Any material such as straw, sawdust, leaves, plastic film, loose soil, etc., that is spread on the surface of the soil to protect the soil and plant roots from the effects of raindrops, soil crusting, freezing, and evaporation, or to control weeds.

Mutagenic - Capable of causing genetic changes.

Nastic movement – Movement of a flat plant part (as a leaf or bud scale) that is oriented in respect to the plant rather than an external source of stimulation, is brought about by disproportionate growth or increase of turgor in the tissues of one surface of the part, and typically involves a curling or bending outward or inward of the whole part in a direction away from the more active surface.

Necrosis - Localized death of tissue usually characterized by browning and desiccation.

Neutral soil - A soil in which the surface layer, at least to normal plow depth, is neither acid nor alkaline in reaction. See **Acid soil, Alkaline soil, Soil pH,** and **Soil reaction.**

Niche - The functional role of an organism in an ecosystem.

Non-selective herbicide - An herbicide that is generally toxic to all plants treated. Some selective herbicides may become non-selective if used at very high rates.

Non-target species - A species not intentionally affected by a pesticide.

No-till - Planting crop seed directly into stubble or sod with no more soil disturbance than is necessary to get the seed into the soil.

Noxious weed - A plant regulated or identified by law as being undesirable, troublesome, and difficult to control. Precise definition varies according to legal interpretations.

Nyctinasty – A nastic movement (as the opening and closing of some flowers) that is associated with diurnal changes of temperature or light intensity.

Oncogenic - Capable of producing or inducing tumors in animals, either benign (non-cancerous) or malignant (cancerous).

Organic soil - A soil that contains a high percentage (>15 or 20%) of organic matter throughout the upper and most weathered part of the soil profile (solum).

Overtop application - A broadcast or banded application applied over the canopy of crops such as by airplane or a raised spray boom of ground equipment.

Peat soil - An organic soil containing more than 50% organic matter. Used in the United States to refer to the stage of decomposition of the organic matter, ‘peat’ referring to the slightly decomposed or undecomposed deposits and ‘muck’ to the highly decomposed materials.

Pelleted formulation - A dry formulation consisting of discrete particles usually larger than 10 cubic millimeters and designed to be applied without a liquid carrier.

Persistent herbicide - A herbicide that, when applied at the recommended rate, will harm susceptible crops planted in normal rotation after harvesting the treated crop, or that interferes with regrowth of native vegetation in non-crop sites for an extended period of time. See residual herbicides.

Pesticide interaction - The action or influence of one pesticide upon another and the combined effect of the pesticide(s) on the pest(s) or crop system.

Phenotype - The characteristics of an organism as determined by the interaction of its genetic constitution and the environment.

Phloem - The living tissue in plants that functions primarily to transport metabolic compounds from the site of synthesis or storage to the site of utilization.

Phytotoxic - Injurious or lethal to plants.

Plant growth regulator - A substance used for controlling or modifying plant growth processes without severe phytotoxicity.

Population - In ecology, a group of individuals of any one species.

Postemergence (POST) - (1) Applied after emergence of the specified weed or crop. (2) Ability to control established weeds.

Preemergence (PRE) - (1) Applied to the soil before emergence of the specified weed or crop. (2) Ability to control weeds before or soon after they emerge.

Preplant application - Applied before planting or transplanting a crop, either as a foliar application to control existing vegetation or as a soil application.

Preplant incorporated (PPI) - Applied and blended into the soil before seeding or transplanting, usually by tillage.

Rate - For herbicides, the quantity of active ingredient or parent compound equivalent expressed as moles or mass per unit area of treated surface or per unit volume of the treated environment (for aquatic or vapor applications). Rates expressed as formulated product should not be used in scientific publications.

Recirculating sprayer - A sprayer system with the nozzle aimed at a catchment device that recovers and recirculates herbicide not intercepted by plants.

Registration - The process designated by the Federal Insecticide, Fungicide and Rodenticide Act (FIFRA) and carried out by the Environmental Protection Agency (EPA) by which a pesticide is legally approved for use in the U.S.

Residual herbicide - A herbicide that persists in the soil and injures or kills germinating weed seedlings for a relatively short period of time after application. See **Persistent herbicide.**

Residue - That quantity of an herbicide or metabolite remaining in or on the soil, plant parts, animal tissues, whole organisms, and surfaces.

Resistance - Ability to withstand exposure to a potentially harmful agent without being injured (There is no general agreement as to the distinction between herbicide tolerance and herbicide resistance in plants).

Safener - A substance that reduces toxicity of herbicides to crop plants by a physiological mechanism.

Saline soil - A non-sodic soil containing sufficient soluble salt to impair its productivity. The electrical conductivity of the saturation extract is greater than 2 decisiemens per meter (dS/m) at 25 C.

Sand - (1) A soil separate consisting of particles between 0.05 and 2.00 mm in equivalent diameter. (2) A soil textural class; soil containing 85% or more of sand; percentage of silt plus 1.5 times the percentage of clay shall not exceed 15%.

Sandy clay - A soil textural class; soil containing 35% or more clay and 45% or more sand.

Sandy clay loam - A soil textural class; soil containing 20-35% clay, <28% silt, and 45% or more sand.

Sandy loam - A soil textural class; soil containing either 20% clay or less, and the percentage of silt plus twice the percentage of clay exceeds 30%, and 52% or more sand; or <7% clay, <50% silt, and 43 to 52% sand.

Seed protectant - (1) A substance applied to seed before planting to control pests. (2) A substance applied to seed to prevent injury from herbicides by a physical mechanism such as adsorption.

Selective herbicide - A chemical that is more toxic to some plant species than to others.

Silt - (1) A soil separate consisting of particles between 0.05 and 0.002 mm in equivalent diameter. (2) A soil textural class; soil containing 80% or more silt and <12% clay.

Silt loam - A soil textural class; soil containing 50% or more silt and 12-27% clay or it contains 50-80% silt and <12% clay.

Silty clay - Soil textural class; soil containing 40% or more clay and 40% or more silt.

Silty clay loam - A soil textural class; soil containing 27-40% clay and <20% sand.

Soil amendment - Any substance added to the soil that alters soil properties. Examples are gypsum, lime, fertilizers, sawdust, etc.

Soil buffer compounds - The clay, organic matter, and compounds such as carbonates and phosphates that enable the soil to resist appreciable change in pH.

Soil bulk density - The mass of dry soil per unit bulk volume. The bulk volume is determined before drying to constant weight at 105 C.

Soil class - A group of soils having a definite range in a particular property such as acidity, degree of slope, texture, structure, land-use capability, degree of erosion or drainage. See **Soil texture** and **Soil structure.**

Soil fertility - The status of a soil with respect to its ability to supply the nutrients essential to plant growth.

Soil injection - Placement of the herbicide beneath the soil surface with a minimum of mixing or stirring of the soil as with an injection blade, knife, or tine.

Soil-layered - Placement of the herbicide beneath the soil surface in a continuous layer with a minimum of mixing.

Soil organic matter - The organic fraction of the soil: includes plant and animal residues at various stages of decomposition, cells and tissues of soil organisms, and substances synthesized by the soil population. Usually determined on soils that have been sieved through a 2.0-mm sieve. See **Humus.**

Soil pH - The negative logarithm of the hydrogen-ion concentration of a soil. The degree of acidity (or alkalinity) of a soil as determined by means of a glass, quinhydrone, or other suitable electrode or indicator at a specified moisture content or soil-water ratio, and expressed in terms of the pH scale.

Soil reaction - The degree of acidity or alkalinity of a soil, usually expressed as a pH value. Descriptive terms commonly associated with certain ranges in pH are: extremely acid <4.5; very strongly acid, 4.5-5.0; strongly acid, 5. 1-5.5; moderately acid, 5.6-6.0; slightly acid, 6. 1-6.5; neutral, 6.6-7.3; slightly alkaline, 7.4-7.8; moderately alkaline, 7.9-8.4; strongly alkaline, 8.5-9.0; and very strongly alkaline, >9.1.

Soil separates - Mineral particles, <2.0 mm in equivalent diameter, ranging between specified size limits. The names and size limits of separates recognized in the United States are: very coarse sand, 2.0-1.0 mm; coarse sand, 1.0-0.5 mm; medium sand, 0.5-0.25 mm; fine sand, 0.25-0.10 mm; very fine sand, 0.10-0.05 mm; silt, 0.05-0.002 mm; and clay, <0.002 mm.

Soil structure - The combination or arrangement of primary soil particles into secondary particles units, or peds. These secondary units may be, but usually are not, arranged in the profile in such a manner as to give a distinctive characteristic pattern. The secondary units are characterized and classified on the basis of size, shape, and degree of distinctness into classes, types, and grades, respectively.

Soil texture - The relative proportions of the various soil separates in a soil as described by the classes of soil texture: sand, loamy sand, sandy loam, loam, silt loam, silt, sandy clay loam, clay loam, silty clay loam, sandy clay, and clay. Textural classes may be modified by the addition of suitable adjectives when coarse fragments are present in substantial amounts; for example, “stony silt loam”, or “silt loam, stony phase”. The sand, loamy sand, and sandy loam are further subdivided on the basis of the proportions of the various sand separates present.

Soil type - The lowest unit in the natural system of soil classification; a subdivision of a soil series and consisting of or describing soils that are alike in all characteristics including the texture of the A horizon.

Soluble concentrate - A liquid formulation that forms a solution when added to water. See Abbreviations and Symbols section for the official GTFAP definition used elsewhere in this handbook.

Soluble granule - A dry granular formulation that forms a solution when added to water. See Abbreviations and Symbols 5cc-tion for the official GIFAP definition used elsewhere in this handbook.

Soluble powder - A dry formulation that forms a solution when added to water. See Abbreviations and Symbols section for the official GIFAP definition used elsewhere in this handbook.

Solum (plural: sola) - The upper and most weathered part of the soil profile; the A and B horizons.

Solution - A homogeneous or single phase mixture of two or more substances.

Spot treatment - A herbicide applied to restricted area(s) of a whole unit; i.e., treatment of spots or patches of weeds within a larger field.

Spray drift - Movement of airborne spray from the intended area of application.

Submersed plant - An aquatic plant that grows with all or most of its vegetative tissue below the water surface.

Surface soil - The uppermost part of the soil ordinarily moved in tillage, or its equivalent in uncultivated soils and ranging in depth from

8 or 10 cm to 20 or 25 cm. Frequently designated as the “plow layer”, the “AP layer”, or the “AP horizon”.

Surfactant - A material that improves the emulsifying, dispersing, spreading, wetting or other properties of a liquid by modifying its surface characteristics.

Susceptibility - The sensitivity to or degree to which a plant is injured by a herbicide treatment.

Suspension - A mixture containing finely divided particles dispersed in a solid, liquid, or gas.

Symplast - The total mass of continuous living cells in a plant connected by plasmodesmata and including the phloem.

Synergism - An interaction of two or more factors such that the effect when combined is greater than the predicted effect based on the response to each factor applied separately.

Synergist - For herbicides; a non-herbicidal compound used to increase the phytotoxicity of an herbicide by a physiological mechanism.

Systemic - Synonymous with translocated herbicide, but more correctly used to describe the property of insecticides or fungicides that penetrate and disperse throughout a plant.

Tank-mix combination - Mixing of two or more pesticides or agricultural chemicals in the spray tank at the time of application.

Teratogenic - Capable of producing birth defects.

Tiller or Tillering - A growth stage of grasses (including cereal crops) when additional shoots are developing from the crown.

Tolerance - (1) Ability to continue normal growth or function when exposed to a potentially harmful agent (there is no general agreement as to the distinction between herbicide tolerance and herbicide resistance in plants). (2) The concentration of a pesticide residue that is allowed in or on raw agricultural commodities as established by the Environmental Protection Agency.

Toxicity - The quality or potential of a substance to cause injury, illness, or other undesirable effects.

Toxicology - The study of the principles or mechanisms of toxicity.

Trade name - A trademark or other designation by which a commercial product is identified.

Translocated herbicide - An herbicide that is moved within the plant. Translocated herbicides may be either phloem mobile or xylem mobile. However, the term frequently is used in a more restrictive sense to refer to herbicides that are applied to the foliage and move downward through the phloem to underground parts.

Vapor drift - The movement of pesticides as vapor from the area of application after the spray droplets have impinged on the target.

Water content - The amount of water lost from the soil upon drying to constant weight at 105 C; expressed as either the mass of water per unit mass of dry soil or as the volume of water per unit bulk volume of soil.

Weed - Any plant that is objectionable or interferes with the activities or welfare of man.
Weed control - The process of reducing weed growth and/or infestation to an acceptable level.

Weed eradication - The elimination of all vegetative plant parts and viable seeds of a weed from a site.

Wetting agent - (1) A substance that serves to reduce the interfacial tensions and causes spray solutions or suspensions to make better contact with treated surfaces (see surfactant). (2) A substance in a wettable powder formulation that causes it to wet readily when added to water.

Wettable powder (WP) - A finely divided dry formulation that can be readily suspended in water. See Abbreviations and Symbols section for the official GIFAP definition used elsewhere in this handbook.

Xylem - The non-living tissue in plants that functions primarily to conduct water and mineral nutrients from roots to the shoot.

CONVERSION FACTORS

Multiply	By	To Obtain
Acre (A)		
A	43,560	ft^2
A	0.40468564	ha
A	4,046.85642	m^2
A	160	rod^2
A	4,840	yd^2
A-ft	1,233.4814	m^3
A-inch	102.7903	m^3
Angstrom (A)		
A	1x10^{-8}	cm
A	3.937008x10^{-9}	inch
Are		
are	100	m^2
Bar		
bar	0.9869233	atm
bar	75.0062	cm Hg at 0 C
bar	1,000,000	dyne/cm^2
bar	1,019.716	g/cm^2
bar	29.53	inches Hg at 0 C
bar	0.001	J/kg
bar	14.5038	lb/inch^2
bar	100	kPa
Barrel (bbl), imperial		
bbl	4.5	bu, imp
bbl	163.655	L
Barrel, US dry		
bbl	7056	inch^3
bbl	0.11563	m^3
bbl	105	qt, US dry
Barrel, US liquid		
bbl	119.2371	L
Bushel (bu), imperial		
bu	36368.7	cm^3
bu	1.28435	ft^3
Bushel, US		
bu	35239.07	cm^3
bu	1.2445	ft^3
Centimeter (cm)		
cm	0.0328084	ft
cm	0.3937008	inch
cm/s	1.968504	ft/mm
cm/s	0.0328084	ft/s
cm/s	0.02236936	mile/h or mph
cm^2	0.1550003	inch^2
cm^3	0.004227	cup, US
cm^3	0.033814	fl oz, US
cm^3	0.06102374	inch^3
cm^3	0.00087988	qt, imp liq
cm^3	0.00105669	qt, US liq
cm^3	1	mL

Multiply	By	To Obtain
Cup, US		
cup	236.588	cm^3
cup	8	fl oz,
Degree Celsius		
C	9/5(C) + 32	F
Degree Fahrenheit		
F	5/9(F - 32)	C
Foot (ft)		
ft	30.48	cm
ft	12	inch
ft	0.3048	m
ft/s	1.09728	km/h
ft/s	18.288	m/min
ft^2	929.0304	cm^2
ft^2/A	0.022957	m^2/ha
ft^3	28,316.847	cm^3
ft^3	1,728	inch^3
ft^3	6.228835	gal, imp liq
ft^3	7.480519	gal, US liq
ft^3	28.316847	L
ft^3	0.0283168	m^3
ft^3	29.922078	qt, US liq
ft^3/min	471.94744	cm^3/s
ft^3/min	0.1038 14	gal/s, imp liq
ft^3/min	0.124675	gal/s, US liq
Gallon (gal), imperial liquid		
gal	4546.09	cm^3
gal	160	fl oz, imp liq
gal	1.20095	gal, US liq
gal	4.54609	L
gal/A	11.23363	L/ha
gal/1000 ft^2	4.79737	L/100m^2
gal/min	0.002675	ft^3/s
gal/min	0.075768	L/s
gal/min	0.272765	m^3/s
Gallon, US dry		
gal	0.125	bu, US
gal	268.8025	inch^3
Gallon, US liquid		
gal	128	fl oz, US
gal	0.1336806	ft^3
gal	0.832674	gal, imp liq
gal	0.859367	gal, dry
gal	231	inch^3
gal	3.785412	L
gal	8	pt, US liq
gal	4	qt, US liq
gal/A	9.3539577	L/ha
gal/1000 ft^2	4.0745837	L/100 m^2
gal/min	0.00222801	ft^3/s
gal/min	0.0630902	L/s
gal/min	0.2271247	m^3/h

Multiply	By	To Obtain
Gallon, US, water in air at 760 mm Hg		
gal	3780.543	g at 0 C
gal	3777.962	g at 15 C
gal	3774.653	g at 20 C
gal	3770.34	g at 25 C
gal	8.33467	lb at 0 C
gal	8.32897	lb at 15 C
gal	8.32167	lb at 20 C
gal	8.31217	lb at 25 C
Gram (g)		
g	0.002204623	lb avdp
g	0.03527396	oz avdp
g	1,000,000	ton, metric
g/cm^3	62.427961	lb avdp/ft^3
g/cm^3	0.03612729	lb avdp/inch^3
g/cm^3	10.02241	lb avdp/gal, imp liq
g/cm^3	8.345404	lb avdp/gal, US liq
g/ha	0.0142749	oz avdp/A
g/L	0.1603586	oz avdp/gal, imp liq
g/L	0.1335265	oz avdp/gal, US liq
g/L	1,000	ppm
g/L	0.062428	lb avdp/ft^3
g/100 ft^2	0.9603	lb avdp/A
g/100 m row	0.0107516	oz avdp/100 ft row
g/m^2	0.3277058	oz avdp/ft^2
g/m^2	0.0294935	oz avdp/yd^2
g/100 m^3	0.00999885	oz avdp/1000 ft^3
Hectare (ha)		
ha	2.471054	A
ha	100	are
ha	107,639.1	ft^2
ha	10,000	m^2
ha-m	8.10713	A-ft
Inch (in)		
inch	2.54	cm
inch	1,000	mil
inch^2	6.4516	cm^2
inch^3	16.387064	cm^3
inch^3	0.576744	fl oz, imp
inch^3	0.5541126	fl oz,US
inch^3	0.003604652	gal, impliq
inch^3	0.004329004	gal, US liq
inch^3	0.017316	qt, US liq
Kilogram (kg)		
kg	2.2046226	lb avdp
kg	35.273962	oz avdp
kg	0.01	quintal
kg/ha	0.892 179	lb avdp/A
kg/ha	14.274866	oz avdp/A
kg/ha	0.02048 16	lb avdp/1000 ft^2
kg/ha	0.0327706	oz avdp/100 ft^2
kg/L	8.345405	lb avdp/gal, US
kg/100L	1.0022413	lb avdp/10 gal, imp
kg/100 L	0.8345405	lb avdp/10 gal, US
kg/100 m row	0.6719771	lb avdp/100 ft row
kg/l100 m^3	0.6242796	lb avdp/1000 ft^3
kg/m^3	0.06242796	lb avdp/ft^3
kg/m^3	0.9988473	oz avdp/ft^3

Multiply	By	To Obtain
Kilometer (km)		
km	3,280.84	ft
km	0.62137119	mile, statute
km	1,093.613	yd
Liter (L)		
L	33.81402	fl oz, US
L	0.03531467	ft^3
L	0.21996925	gal, imp liq
L	0.26417205	gal, US liq
L	61.023744	inch^3
L	1.056688	qt, US liq
L/A	0.0060646	gal/1000 ft^2, US liq
L/ha	0.089018	gal/A, imp liq
L/ha	0.106907	gal/A, US liq
L/ha	0.712147	pt/A, imp liq
L/ha	0.855253	pt/A, US liq
L/100 m^2	0.208448	gal/1000 ft^2, imp liq
L/100 m^2	0.245424	gal/1000 ft^2, US liq
L/100 m^2	1.634865	pt/1000 ft^2, imp liq
L/100 m^2	1.963391	pt/1000 ft^2, US liq
L/min	2.11888	ft^3/h
L/min	13.19815	gal/h, imp liq
L/min	15.85032	gal/h, US liq
Meter (m)		
m	3.2808399	ft
m	39.3700787	in
m	1.0936133	yd
m/s	196.85039	ft/min
m/s	2.2369363	mile/h, statue
m^2	10.76391	ft^2
m^2	1,550.0031	inch^2
m^2	1.19599	yd^2
m^3	0.0008107	A-ft
m^3	35.314667	ft^3
m^3	264.17205	gal, US liq
m^3	1,000	L
m^3	1.307951	yd^3
Mile, statute		
mile	5,280	ft
mile	1.609344	km
mile	0.868976	mile, naut., or int.
mile	1,760	yd
mile^2	640	A
mile^2	2258.998811	ha
mile^2	2.58998811	km^2
mile/h	88	ft/min
mile/h	1.466667	ft/s
mile/h	1.609344	km/h
mile/h	26.8224	m/min
Mile, nautical or international		
mile	6,076.11549	ft
mile	1.852	km
mile	1.150779	mile, statute
Milligram (mg)		
mg/kg	0.4535923	mg/lb avdp
mg/lb avdp	2.204623	mg/kg
Milliliter (mL)		
mL	0.610237	inch^3

Multiply	By	To Obtain
mL/10,000 L	0.016	fl oz/1000 gal, imp liq
mL/10,000 L	0.0128	fl oz/l000 gal, US liq
Ounce (oz), avoirdupois (avdp)		
oz avdp	28.349523	g
oz avdp	0.0625	lb avdp
oz avdp/A	70.053204	g/ha
oz avdp/ 100 ft row	93.00912	g/100 m row
oz avdp/ft^2	305.1517	g/m^2
oz avdp/yd^2	33.90575	g/m^2
oz avdp/ft^3	1.001154	kg/m^3
oz avdp/1000 ft^3	100.01154	g/100 m^3
oz avdp/gal, imp liq	6.23602	g/L
oz avdp/gal, US liq	7.48915	g/L
Ounce, fluid imperial		
fl oz	0.96076	fl oz, US liq
fl oz	28.41306	mL
fl oz/1000 gal, imp liq	62.5	mL/10,000 L
Ounce, fluid US		
fl oz	29.57353	cm^3
fl oz	0.125	cup, US liq
fl oz	1.0408428	fl oz, imp liq
fl oz	29.57353	mL
fl oz	0.03125	qt, US liq
fl oz	2	tbs
fl oz/A	73.0778	mL/ha
fl oz/1000 gal, US liq	78.125	mL/10,000 L
Parts per million (ppm)		
ppm	8.32897	lb avdp/1,000,000 gal, US, water at 15˚C at 760 mm Hg. See Gallon, US, water.
Pascal (see Bar)		
kPa	0.145038	psi
Pa	10	dyne/cm^2
Pa	1	newton/m^2
Pa	0.00750062	mmHg or Torr
Pint (pt), imperial liquid		
pt	20	fl oz, imp liq
pt	1.20095	pt, US liq
pt/A	1.404204	L/ha
pt/1000 ft^2	0.611671	L/100m^2
Pint, US dry		
pt	550.61047	cm^3
pt	33.600312	inch^3
pt	0.145456	gal, US liq
pt	550.595	mL

Multiply	By	To Obtain
Pint, US liquid		
pt	473.1765	cm^3
pt	2	cup
pt	16	fl oz, US liq
pt	0.125	gal,US liq
pt	28.875	inch^3
Pint, US liquid con't		
pt	473.1765	mL
pt	0.8326742	pt, imp liq
pt	0.5	qt, US liq
pt/A	1.169245	L/ha
pt/1000 ft^2	0.509323	L/100 m^2
pt/1000gal	1.25	L/10,000 L
Pound (lb), avoirdupois		
lb	453.59237	g
lb	16	oz avdp
lb/A	1.0413	g/100 ft^2
lb/A	1.120851	kg/ha
lb/A	0.022957	lb/b000 ft^2
lb/A	0.03673	oz avdp/100 ft^2
lb/100 ft row	1.48815	kg/100 m row
lb/1000 ft^2	488.2428	g/100 m^2
lb/1000 ft^2	43.5597	lb/A
lb/1000 ft^2	48.8243	kg/ha
lb/ft^3	0.0160185	g/cm^3
lb/ft^3	16.01846	g/L
lb/1000 ft^3	1.60185	kg/100 m^3
lb/gal, imp liq	99.77637	g/L
lb/gal, US liq	119.8264	g/L
lb/gal, US liq	0.119826	kg/L
lb/gal, US liq	7.480519	lb/ft^3
lb/inch^2	0.068046	atm
lb/inch^2	0.0689476	bar
lb/inch^2	6.89476	kPa
Quart (qt), imperial liquid		
qt	1136.5225	mL
qt	1.20095	qt, US liq
Quart, US liquid		
qt	946.35295	cm^3
qt	32	fl oz, US liq
qt	0.25	gal, US liq
qt	*57.75*	inch^3
qt	946.35295	mL
qt	2	pt, US liq
qt	0.832674	qt, imp liq
qt/A	2.3385	L/ha
Quintal (q)		
q	220.46226	lb avdp
q	100	kg
q	10	ton, metric
q/ha	89.20607	lb/A
Rod		
rod	16.5	ft
rod	5.0292	m

Multiply	By	To Obtain
Tablespoon (tbs)		
tbs	14.78676	cm^3
tbs	0.0625	cup
tbs	0.5	fl oz, US liq
tbs	3	tsp
Teaspoon (tsp)		
tsp	4.928922	cm^3
tsp	**0.333333**	**tbs**
Ton, long		
ton, long	1,016.0469088	kg
ton, long	2,240	lb avdp
ton, long	1.0 16047	ton, metric
Ton, metric		
ton	1,000	kg
ton	2,204.6226	lb avdp
ton	0.1	quintal
ton	0.9842065	ton, long
ton	1.1023113	ton
ton/ha	892.179	lb avdp/A
ton/ha	0.44609	ton/A
Ton, short		
ton	907.18474	kg
ton	2,000	lb avdp
Ton, short con't		
ton	0.8928571	ton, long
ton	0.9071847	ton, metric
ton/A	2.2417023	ton/ha, metric
Yard (yd)		
yd	91.44	cm
yd	3	ft
yd	0.9144	m
yd^3	0.000619	A-ft
yd^3	168.1786	gal, imp liq
yd^3	201.974	gal, US liq
yd^3	764.5549	L
yd^3	0.7645549	m^3

COMPANY CONTACT INFORMATION

Aceto Agricultural Chemicals Corp.
One Hollow Lane, Suite 201
Lake Success, NY 11042
516-627-6000
www.aceto.com

Advan, LLC (Advan)
300 Colonial Center Parkway,
Suite 230, Roswell, GA 30076 U.S.A.
800-250-5024
www.advanllc.com

Agriliance
P.O. Box 64089, MS 385
St. Paul, MN 55164-0089
800-535-4635
www.agriliance.com

Agway
www.agway.com

Albaugh, Inc./Agri Star
1525 N.E. 36th Street
Ankeny, Iowa 50021
800-247-8013
www.albaughinc.com

Amvac Chemical Corporation (Amvac)
4100 East Washington Blvd.
Los Angeles, CA 90023
888-GO-AMVAC
www.amvac-chemical.com

Applied Biochemists
W 175 N11163 Stonewood Dr., Suite 234
Germantown, WI 53022
800-558-5106
www.appliedbiochemists.com

BASF Ag Products (BASF)
P.O. Box 13528
26 Davis Drive
Research Triangle Park, NC 27709-3528
919-547-2000
www.agproducts.basf.com

Bayer CropScience
2 T.W. Alexander Drive
P.O. Box 12014
Research Triangle Park, NC 27709
919-549-2000
www.bayercropscienceus.com

Cedar Chemical Company (Cedar)
5100 Poplar Avenue
Suite 2414
Memphis, TN 38137
901-685-5348
www.cedarchem.com

Cerexagri, Inc. (Cerexagri)
630 Freedom Business Center
Suite 402
King of Prussia, PA 19406
800-438-6071
www.cerexagri.com

Cheminova, Inc. (Cheminova)
1700 Route 23 North, Suite 210
Wayne, NJ 07470
973-305-6600
www.cheminova.us.com

Chemtura Corporation (Chemtura) (formerly Uniroyal Chemical)
199 Benson Road
Middlebury, CT 06749 USA
203-573-2000
www.chemtura.com

Dongbu Hannong Chemical Co. Ltd.
Dongbu Financial Center 19-22F, 891-10
Daechi-dong
Gangnam-gu
Seoul 135-523, Korea
+82-2-3484-1500
www.dongbuhitek.com

Dow AgroSciences LLC (Dow AgroSciences)
9330 Zionsville Road
Indianapolis, IN 46268
317-337-3000
800-258-3033
www.dowagro.com

Drexel Chemical Company (Drexel)
P.O. Box 13327
1700 Channel Avenue
Memphis, TN 38113
901-774-4370
www.DrexChem.com

E.I. du Pont de Nemours and Company Co., Inc. (Du Pont)
Crop Protection
Laurel Run Building, Chestnut Run Plaza
Wilmington, DE 19898
1-888-6-DUPONT
1-888-638-7668
www.cropprotection.dupont.com

FMC Corporation (FMC)
Agricultural Products Group
1735 Market Street
Philadelphia, PA 19103
215-299-6000
cropsolutions.fmc.com

Gharda Chemicals Limited (Gharda)
5/6, Jer Mansion,
W.P. Warde Road, Off Turner Road.
Bandra West.
Mumbai-400050
India
Tel: +91 22 26452492/ 26422230/ 26430654
www.gharda.com

Gowan Company (Gowan)
P.O. Box 5569
Yuma, AZ 85366-5569
800-883-1844
www.gowanco.com

Griffin LLC (Griffin)
P.O. Box 1847
Valdosta, GA 31603
229-242-8635
www.griffinllc.com

Helena Chemical Company (Helena)
225 Schilling Blvd., Suite 300
Collierville, TN 38017
901-761-0050
www.helenachemical.com

Helm Agro US, Inc. (Helm Agro)
8295 Tournament Drive, Suite 310
Memphis, TN 38125
901-312-1525
www.helmagro.com

J.R. Simplot Company/Plant Health Technologies (J.R. Simplot)
P.O. Box 70013
Boise, ID 83707
208-672-2700
www.simplot.com

KMG Chemical (KMG)
10611 Harwin Drive, Suite 402
Houston, TX USA 77036-1534
713-600-3850
www.kmgchemicals.com

Kumiai Chemical Industry Co., Ltd. (Kumiai)
4-26, Ikenohata 1-chome
Taito-ku
Tokyo 110-8782, Japan
03-3822-5036
www.kumiai-chem.co.jp
Kwizda
www.kwizda.at

Lebanon Chemical Corporation (Lebanon)
10413 River Landing Rd.
Denton, MD, 21629
410-479-2030

LG Chemical (LG)
LG Chem Headquarters
LG Twin Towers 20,
Yeouido-doing
Yeongdeungpo-gu
Seoul 150-721, Korea

Adama (Formerly MANA - Makhteshim Agan of North America, Inc. (Makhteshim Agan))
4515 Falls of Neuse Road
Suite 300
Raleigh NC 27609
919-256-9300
www.manainc.com

Micro Flo Products (Micro Flo or Arysta Life Science)
530 Oak Court Drive
Suite 100
P.O. Box 772099
Memphis, TN 38117-2099
901-432-5000
www.microflocompany.com

Mitsubishi Chemical Corporation (Mitsubishi)
Group Information Center
+81(0)3-6414-3000
www.m-kagaku.co.jp

Monsanto Company (Monsanto)
800 North Lindbergh Blvd.
St. Louis, MO 63167
314-694-1000
www.monsanto.com/monsanto/us_ag

Monterey AgResources
P.O. Box 35000
Fresno, CA 93745-5000
559-499-2100
www.montereyagresources.com

Nichino America, Inc.
4550 New Linden Hill Road, Suite 501
Wilmington, DE 19808
302-636-9001
www.nichino.net

Nissan Chemical America Corporation (Nissan)
10777 Westheimer
Suite 830
Houston, TX 77042
www.nissanchem.us

Nufarm Americas, Inc. (Nufarm)
150 Harvester Drive, Suite 200
Burr Ridge, IL 60527
800-345-3330
www.us.nufarm.com

Pro-Serve, Inc. (Pro-Serve)
400 E. Brooks Rd.
Memphis, TN 38109
www.pro-serveinc.com

PBI Gordon Corporation (PBI Gordon)
1217 W. 12th Street
Kansas City, MO 64101
816-421-4070
www.pbigordon.com

Phelps Dodge Corporation (Phelps Dodge)
P.O. Box 20001
El Paso, TX 79998
800-223-8567
www.phelpsdodge.com

PROKoZ, Inc. (PROKoZ)
100 North Point Center East Ste. 330
Alpharetta GA 30022
770-619-9832
www.prokoz.net

Scotts
Scotts Consumer Service
14111 Scottslawn Road
Marysville, OH 43041
www.scotts.com

Sipcam Agro USA, Inc. (Sipcam Agro)
300 Colonial Center Parkway, Suite 230
Roswell, GA 30076
770-587-1032
www.sipcamagrousa.com

SePRO Corporation (SePRO)
11550 North Meridian Street
Suite 600
Carmel, IN 46032 USA
317-580-8282
www.sepro.com

Solvay Duphar B.V. (Solvay Duphar)
C.J. van Houtenlaan 36
P.O. Box 900
1380 DA Weesp
The Netherlands

Sumitomo Chemical (Sumitomo)
Tokyo Sumitomo Twin Building (East),
27-1, Shinkawa 2-chome,
Chuo-ku, Tokyo 104-8260, Japan
+81-3-5543-5500
www.sumitomo-chem.co.jp

Syngenta Crop Protection, Inc. (Syngenta Crop Protection)
P.O. Box 18300
Greensboro, NC 27419
336-632-6000
www.syngentacropprotection-us.com/

Taminco, Inc. (Taminco)
2000 Lake Park Drive
Smyrna, GA 30080
800-426-3820
www.taminco.com

Tenkoz, Inc. (Tenkoz)
100 North Point Center East, Suite 330
Alpharetta, GA 30022
770-343-8509
www.tenkoz.com

Tokuyama
Shibuya Konno Bldg.
3-3-3, Shibuya
Shibuya-ku, Tokyo 150-8383 Japan
www.tokuyama.co.jp

UAP - Loveland Products, Inc. (UAP – Loveland Products)
P.O. Box 1286
Greeley, CO 80632
970-356-4400

www.uap.com
Ube Industries, Inc. (Ube Industries)
northamerica.ube.com

United Phosphorus Inc. (United Phosphorus)
423 Riverview Plaza
Trenton, NJ 08611
609-392-8200
www.upi-usa.com

United Suppliers, Inc. (United Suppliers)
30473 260th Street
Eldora, IA 50627
800-782-5123
www.unitedsuppliers.com

Valent Agricultural Products (Valent)
P.O. Box 8025
Walnut Creek, CA 94596
800-6-VALENT (682-5368)
www.valent.com/

Wilbur-Ellis Company (Wilbur-Ellis)
PO Box 1286
Fresno, CA 93715
559-496-3350
www.wilburellis.com/

Herbicide Company "Genealogy"

September 2013

The following chart is intended to show the history of the major U.S. herbicide companies. The information depends largely on people's memories, which sometimes can be inexact, on records from the headquarters of major companies, and from histories on the internet. No guarantees are made for accuracy, although I think it is pretty close. The dates of the founding of companies or of acquisitions and mergers sometime vary slightly from one reference to another, so they should not be considered as solid historical facts.

Only U.S. companies are listed. International companies are listed only if they had subsidiaries in the U.S., such as Bayer or BASF. I have tried to include mergers or acquisitions of entire companies or the ag divisions of companies, but acquisition of individual products are mentioned only occasionally. In many cases, the major company continues in existence and it is the agricultural division that becomes part of another company. Example: Aventis sold its ag products division to Bayer while the pharmaceutical portion of Aventis continues. Acquisitions of seed companies are not included.

The major companies included are those with a history of synthesis, screening, and development of herbicides in the U.S., even if their parent company is overseas. This excludes marketing companies, post-patent distributors, and those companies dealing only with non-herbicide pesticides. Some companies have a distinguished herbicide history but no longer develop new herbicides. These are so noted.

Numerous companies and individuals have been consulted and have been very helpful. But I have not always followed suggestions exactly if I felt I had more accurate information from a different source, so all the errors and omissions are mine.

Changes will be shown at:

http://cropandsoil.oregonstate.edu/system/files/u1473/tree.pdf

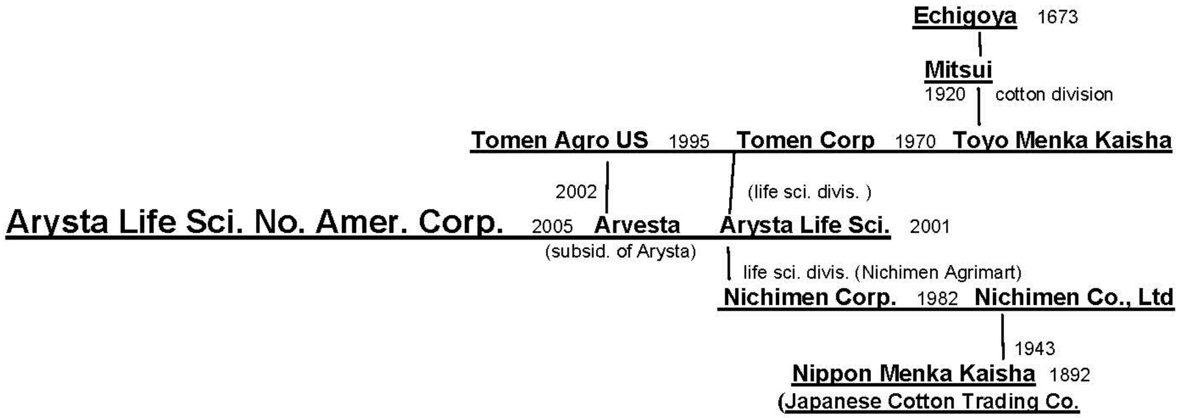
Or e-mail me and I can send you a chart directly.

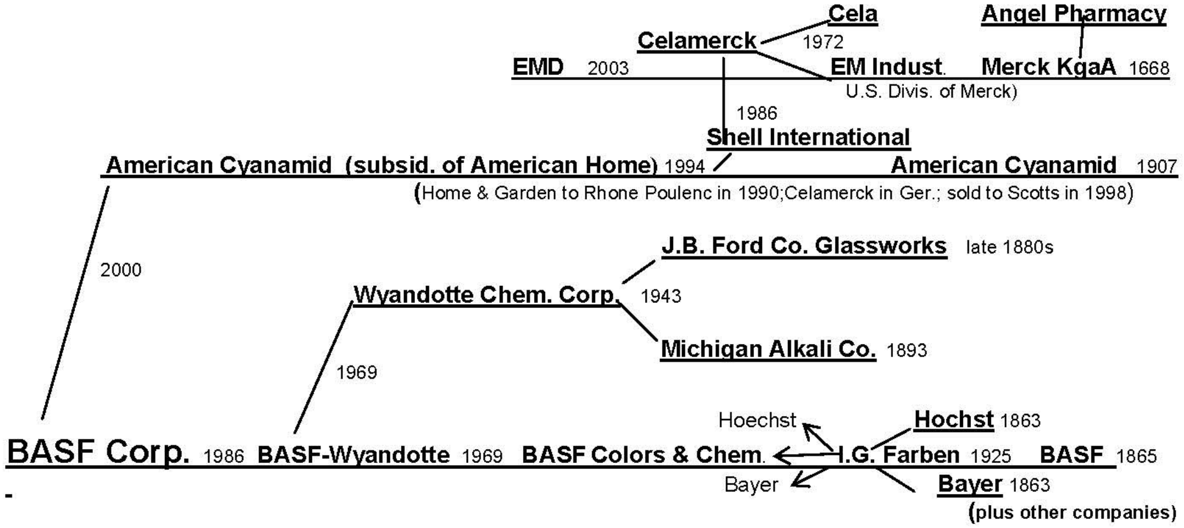
Arnold P. Appleby, Prof. Emeritus
Crop Science, Oregon St. University
Corvallis, OR 97331-3002
Phone: 541/737-5894
arnold.p.appleby@oregonstate.edu

History of the U.S. Herbicide Companies

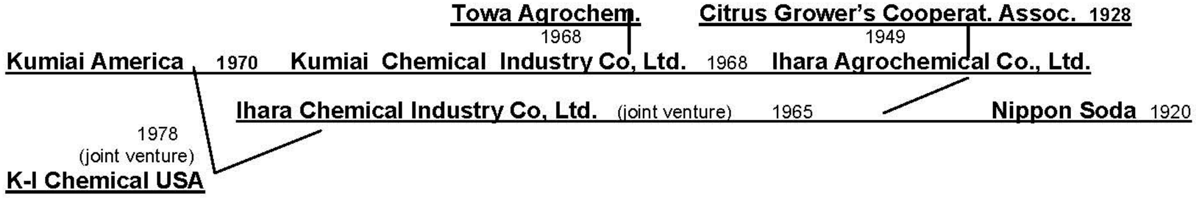
Arnold P. Appleby, Oregon State University

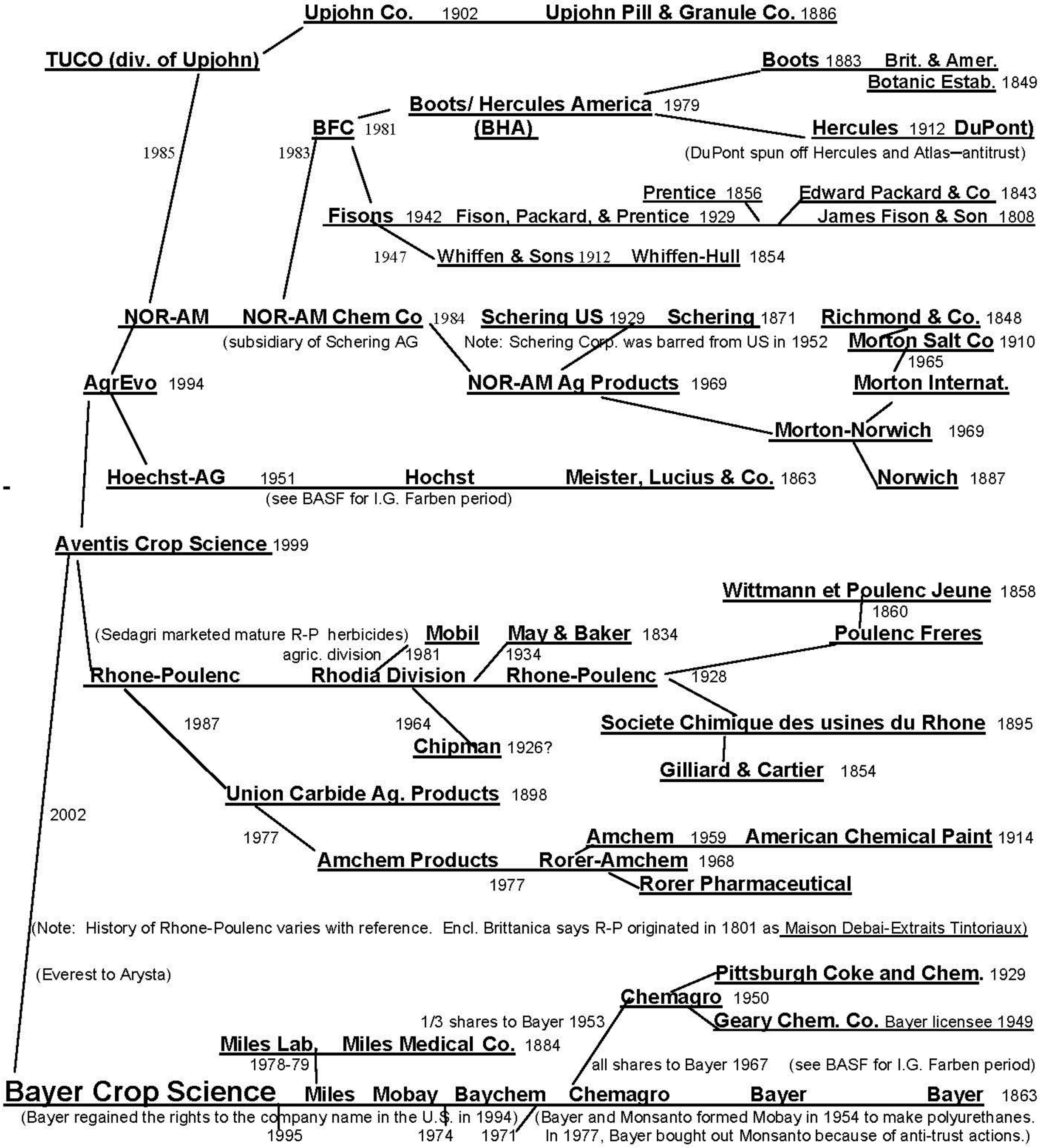
September 2013

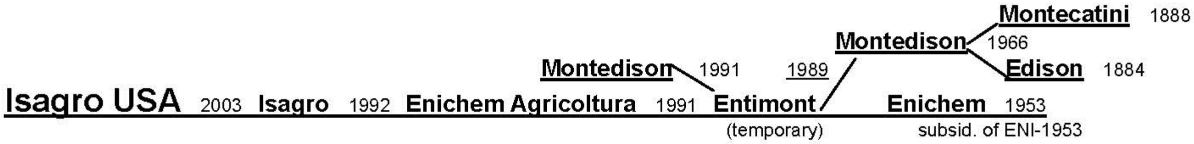


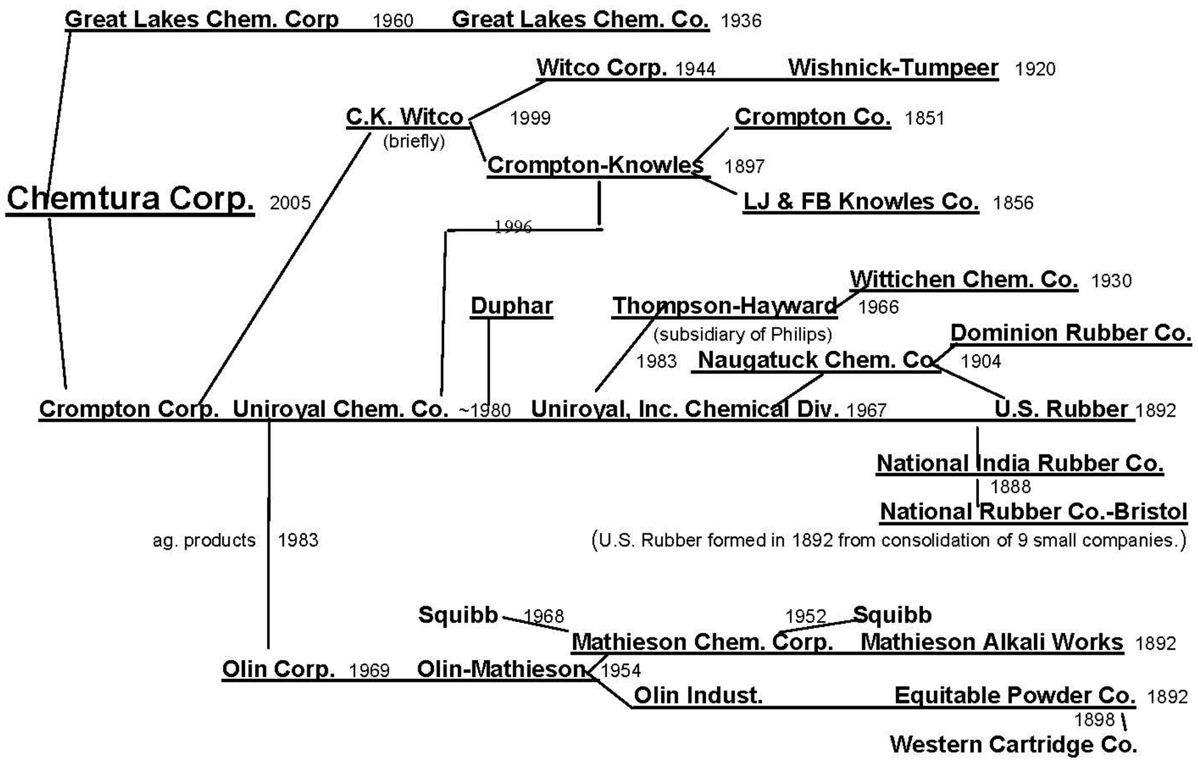


(BASF comes from Badische Anilin & Soda Fabrik)
(I.G.Farben dissolved in 1945 and 12 companies emerged in 1951 including the original three major ones.)
(BASF acquired Sandoz corn herbicides and some personnel-1996 when Sandoz merged w/ Ciba)

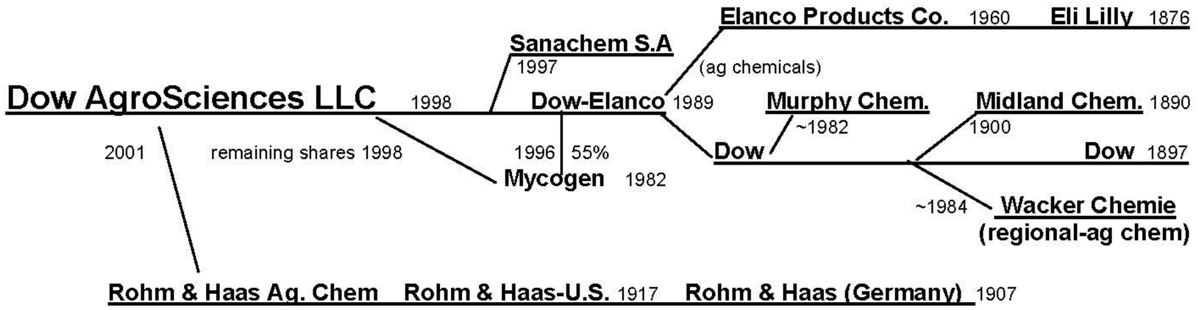


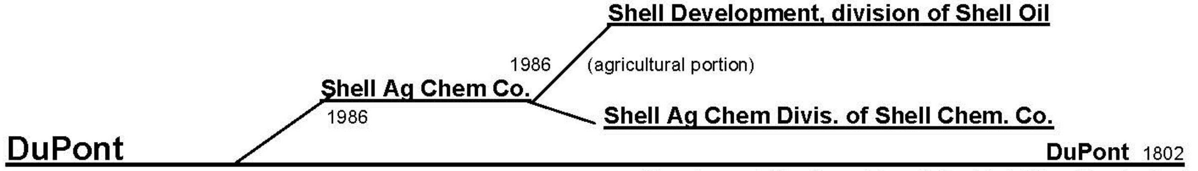

Upjohn Co. 1902 Upjohn Pill & Granule Co. 1886
TUCO (div. of Upjohn)
Boots 1883 Brit. & Amer. Botanic Estab. 1849
Boots/ Hercules America 1979 (BHA)
BFC 1981
Hercules 1912 DuPont)
(DuPont spun off Hercules and Atlas—antitrust)
1985
1983
Prentice 1856
Edward Packard & Co 1843
Fisons 1942 Fison, Packard, & Prentice 1929
James Fison & Son 1808
1947
Whiffen & Sons 1912 Whiffen-Hull 1854
NOR-AM
NOR-AM Chem Co 1984
(subsidiary of Schering AG
Schering US 1929 Schering 1871
Note: Schering Corp. was barred from US in 1952
Richmond & Co. 1848
Morton Salt Co 1910
1965
AgrEvo 1994
NOR-AM Ag Products 1969
Morton Internat.
Morton-Norwich 1969
Hoechst-AG 1951 Hochst Meister, Lucius & Co. 1863
(see BASF for I.G. Farben period)
Norwich 1887
Aventis Crop Science 1999
Wittmann et Poulenc Jeune 1858
1860
(Sedagri marketed mature R-P herbicides)
Mobil agric. division 1981
May & Baker 1834
1934
Poulenc Freres
Rhone-Poulenc
Rhodia Division
Rhone-Poulenc 1928
1987
1964
Societe Chimique des usines du Rhone 1895
Chipman 1926?
Gilliard & Cartier 1854
Union Carbide Ag. Products 1898
2002
1977
Amchem 1959 American Chemical Paint 1914
Amchem Products
Rorer-Amchem 1968
1977
Rorer Pharmaceutical
(Note: History of Rhone-Poulenc varies with reference. Encl. Brittanica says R-P originated in 1801 as Maison Debai-Extraits Tintoriaux)
(Everest to Arysta)
Pittsburgh Coke and Chem. 1929
Chemagro 1950
1/3 shares to Bayer 1953
Geary Chem. Co. Bayer licensee 1949
Miles Lab. Miles Medical Co. 1884
1978-79
all shares to Bayer 1967 (see BASF for I.G. Farben period)
Bayer Crop Science Miles Mobay Baychem Chemagro Bayer Bayer 1863
(Bayer regained the rights to the company name in the U.S. in 1994)
(Bayer and Monsanto formed Mobay in 1954 to make polyurethanes. In 1977, Bayer bought out Monsanto because of anti-trust actions.)
1995 1974 1971


Montecatini 1888
Montedison 1966
Montedison 1991
1989
Edison 1884
Isagro USA 2003 Isagro 1992 Enichem Agricoltura 1991 Entimont Enichem 1953
(temporary)
subsid. of ENI-1953

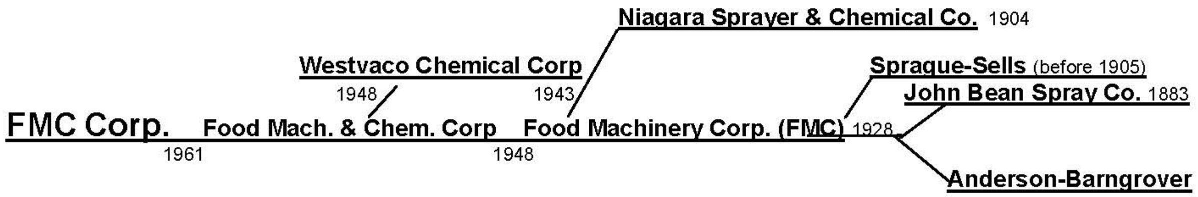


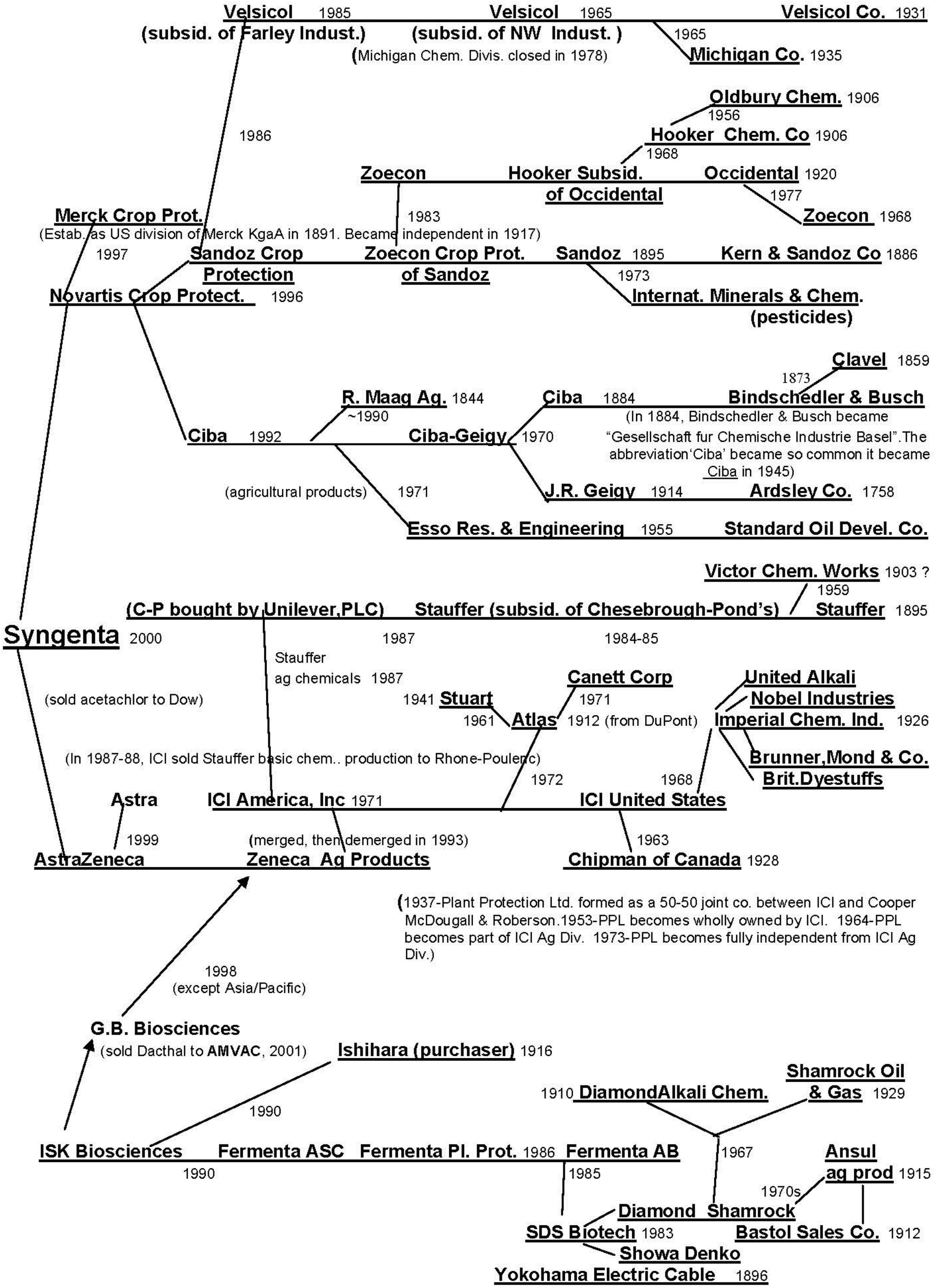
(U.S. Rubber formed in 1892 from consolidation of 9 small companies.)





(Hercules and Atlas formed from DuPont in 1912 anti-trust action)





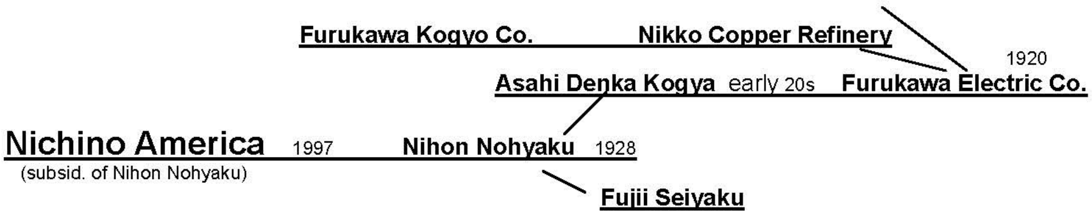
(Michigan Chem. Divis. closed in 1978)

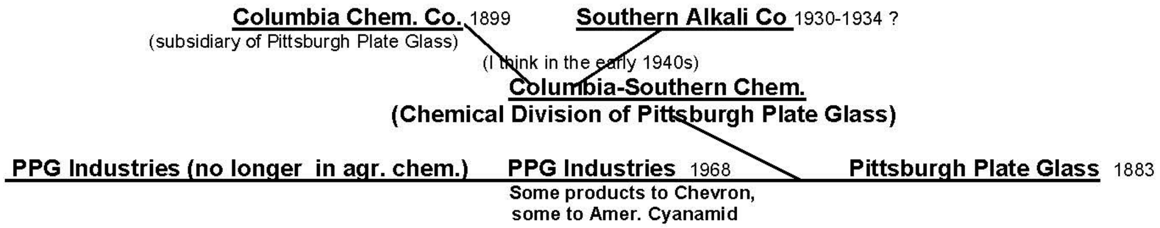
(Estab. as US division of Merck KgaA in 1891. Became independent in 1917)

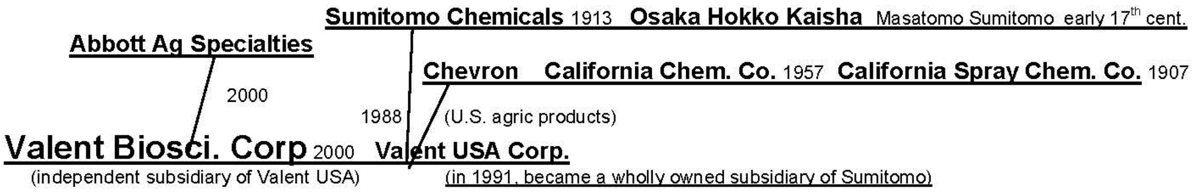
(In 1884, Bindschedler & Busch became "Gesellschaft fur Chemische Industrie Basel".The abbreviation'Ciba' became so common it became Ciba in 1945)

(In 1987-88, ICI sold Stauffer basic chem.. production to Rhone-Poulenc)

(1937-Plant Protection Ltd. formed as a 50-50 joint co. between ICI and Cooper McDougall & Roberson.1953-PPL becomes wholly owned by ICI. 1964-PPL becomes part of ICI Ag Div. 1973-PPL becomes fully independent from ICI Ag Div.)

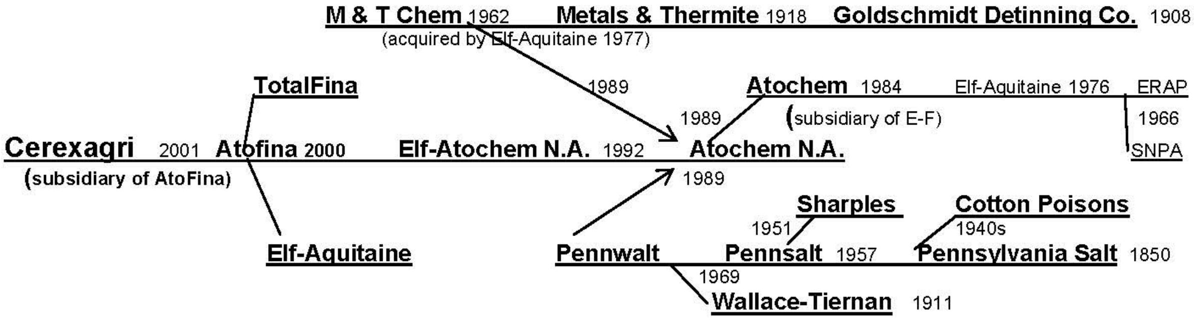


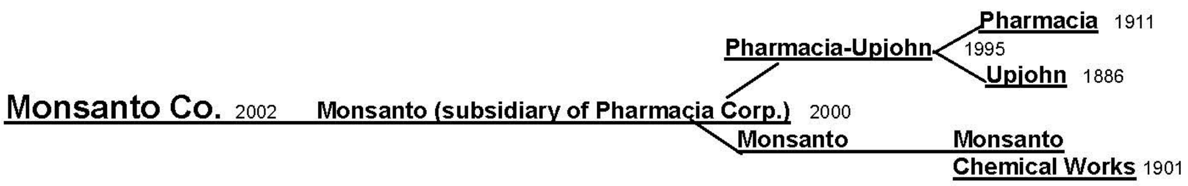




Note: Chevron ex-U.S. agric. products to Tomen Agro. and Rhone Poulenc
Chevron lawn and garden (Ortho) to Monsanto (Solaris Divis. in 1993). These products then sold to Scotts in 1998.

Companies With Herbicide History That No Longer Synthesize and Develop New Herbicides





Other Companies

Besides the 80-some names included in the preceding chart, there were other companies that were once associated with herbicides. Some are still companies, such as PPG, but are no longer in the herbicide business. Some apparently sold any products and ceased to exist. Some perhaps were primarily distributors and owned no products of their own, although I have omitted what I perceive to be strictly marketing companies or herbicide distributors.

Following is a partial list along with examples of products that were associated with them. Please feel free to send me additions or corrections.

Company	Herbicides .
Agrolinz	Sold pyridate to Sandoz in the 1990s.
Air Products	AP-20
Allied Chem. (General Chem. Div.)	HCA. Urox, Urab (Some products to Hopkins → United Ag Products. Since dropped.)
Antara	Primarily wetting agents
Atlas and Hercules	Atlas had Atlacide (later sold by Chipman), Hercules had Herban and Antor. Hercules formed in 1882 jointly by Laflin & Rand and DuPont. Because of antitrust action, Atlas and Hercules were formed from DuPont in 1912. Atlas was purchased by ICI in 1971 and Hercules merged with Boots.
Buckman Labs.	Buban
Esso (Standard Oil of NJ) –ag chem sold to Ciba-Geigy. Name then changed to Exxon.	Stoddart solvent, Tolban sold to Ciba-Geigy.
PBI-Gordon	Originally formed from merger of Private Brands, Inc.and Gordon's Chem. Co. in 1947. Absorbed tech. personnel from Gulf, Thompson-Hayward, and Farmland. Were associated with diclobenil, Embark, et al. Now market phenoxy formulations, primarily for lawn care.
3 M	Destun, Sustar. Embark was sold to PBI-Gordon.
Reichhold	Na PCP
Sharples	Introduced endothall in 1951. Became subsidiary of Pennsylvania Salt Co. in 1951, and their chem. products integrated in 1955.
Spencer → Gulf	Clobber, Outfox, Topcide, Prefox. Carbyne sold to Velsicol.
Sunco	Major supplier of Stoddart Solvent.
Tenneco	TCH-1626. TCH- 1636
U.S. Borax	Borascu, Borolin, Ureabor, Cobex (Some products to Occidental; Cobex now produced by Wacker in Germany)
Vertac	dinoseb, manufactured and distributed several generic chemicals
Vineland	organic arsenicals

Index

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ISBN 978-0-615-98937-2
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