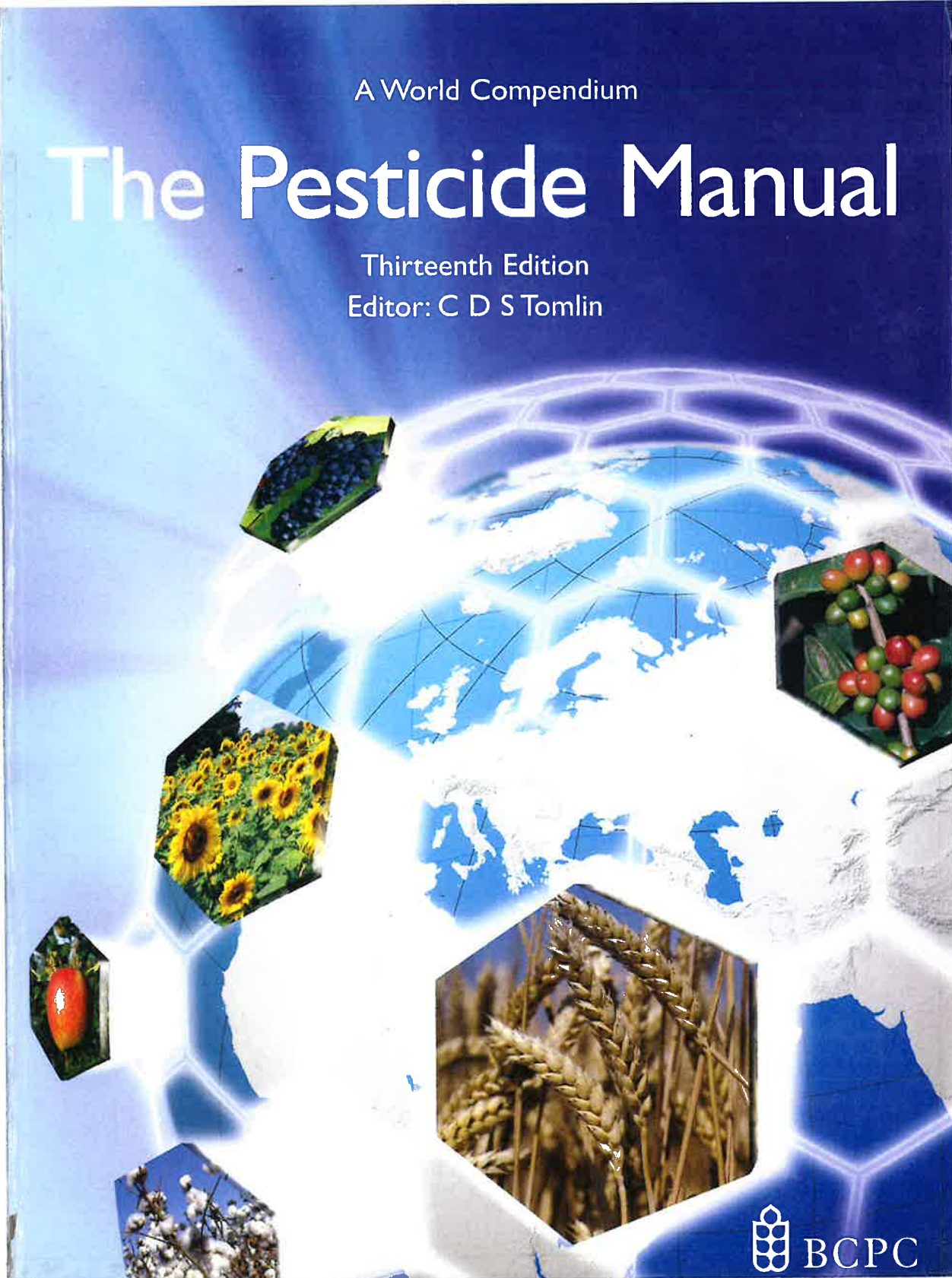


A World Compendium

The Pesticide Manual

Thirteenth Edition
Editor: C D S Tomlin



BCPC



Copyright

© 2003 BCPC (British Crop Protection Council)

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior permission of the copyright owner.

British Library Cataloguing in Publication Data. A catalogue record of this book is available from the British Library.

ISBN 1 901396 13 4

First published	1968	Seventh edition	1983	Thirteenth edition	2003
Second edition	1971	Eighth edition	1987		
Third edition	1972	Ninth edition	1991		
Fourth edition	1974	Tenth edition*	1994		
Fifth edition	1977	Eleventh edition	1997		
Sixth edition	1979	Twelfth edition	2000		

* The tenth edition incorporated *The Agrochemicals Handbook*, previously published by The Royal Society of Chemistry.

Cover design by m360 Nottingham
Typeset and printed by Page Bros., Norwich

Published by: BCPC, 7 Omni Business Centre, Omega Park, Alton, Hampshire, GU34 2QD, UK
Tel +44 (0) 1420 593 200 Fax +44 (0) 1420 593 209
Email: md@bcpc.org Web: www.bcpc.org

All BCPC publications can be bought from: BCPC Publications, 7 Omni Business Centre, Omega Park, Alton, Hampshire, GU34 2QD, UK
Tel +44 (0) 1420 593 200 Fax +44 (0) 1420 593 209
Email: publications@bcpc.org
Or direct from the BCPC Online Book Shop at www.bcpc.org/bookshop

Disclaimer Every effort has been made to ensure that all information in this edition of *The Pesticide Manual* is correct at the time of going to press. However, the editor and the publisher do not accept liability for any error or omission in the content, or for any loss, damage or any other accident arising from the use of the products listed therein.

Before handling, storing or using any approved crop protection product, it is essential to follow the instructions on the label.

PHYSICAL CHEMISTRY: Mol. wt. 381.4 M.f. $B_4H_{10}Na_2O_{17}$ Form Colourless crystalline solid, efflorescent at low r.h. M.p. 742°C (anhydrous sodium tetraborate) S.g./density 1.71 (20°C) Solubility In water 47.1 g/l (pH 9.3, 20°C). Soluble in glycerol and ethylene glycol. Insoluble in ethanol. Stability Stable. When heated above c. 62°C, borax loses water of crystallisation, first forming the pentahydrate and then anhydrous sodium tetraborate. F.p. A fire retardant

COMMERCIALISATION: History Borax has long been used as a mild antiseptic fungicide and as a herbicide. Disodium tetraborate and sodium metaborate were introduced as herbicides by the US Borax & Chemical Corp. Patents US 2998310 (sodium octaborate); US 3032405 (sodium metaborate) Manufacturers Drexel; IMC Chemical; Borax.

APPLICATIONS: Mode of action Non-selective herbicide, causing plants to yellow and desiccate. Uses Total control of vegetation on non-crop land, such as paths, giving long-term control. Also used in insect baits for food stores to control Formicidae. Also applied to tree stumps for control of *Heterobasidion annosum*. Phytotoxicity Not to be used near desired plants. Formulation types WP. Compatibility Its aqueous solution is alkaline and so incompatible with some herbicides. Selected products 'Dehybor' (Borax); 'Pyrobor' (IMC Chemical).

ANALYSIS: Product analysis by acid-base titration (CIPAC Handbook, 1992, E, 376; AOAC Methods, 13th Ed., 20.056). Residues determined by colorimetry, titration, atomic absorption spectroscopy (ibid., 14th Ed., 20.057–20.067; 13th Ed., 20.042–20.045).

MAMMALIAN TOXICOLOGY: Reviews ECETOC Technical Report XXX, 'Toxicology and Risk Assessment of the Inorganic Borates' (1994). Oral Acute oral LD₅₀ for rats 4500–6000 mg/kg. Skin and eye Acute percutaneous LD₅₀ for rabbits >10 000 mg/kg. Not an eye or skin irritant. NOEL (2 y) for rats 154, dogs 78 mg/kg b.w. daily. Other Not carcinogenic, not mutagenic. No reproductive or developmental toxicity noted. Toxicity class WHO (a.i.) U; EPA (formulation) III

ECOTOXICOLOGY: Fish LC₅₀ (24 d) for rainbow trout 1320 mg/l (disodium tetraborate decahydrate). Daphnia LC₅₀ (48 h) 1170 mg/l (disodium tetraborate decahydrate). Bees Not hazardous to bees.

ENVIRONMENTAL FATE: Animals Not metabolised in animals. Soil/Environment No microbial degradation. Disappearance from soil is by washing out. Persistence in soil is ≤2 y, depending on rainfall and soil structure.

87 Bordeaux mixture

Fungicide

FRAC M1; multi-site: inorganic

NOMENCLATURE: Common name Bordeaux mixture (draft E-ISO, accepted in lieu of common name)

IUPAC name A mixture, with or without stabilising agents, of calcium hydroxide and copper(II) sulfate

Chemical Abstracts name Bordeaux mixture

CAS RN [8011–63–0] Bordeaux mixture; [11125–96–5] Burgundy mixture

PHYSICAL CHEMISTRY: Composition Hydrated lime and copper sulfate. Form Fine, green, precipitated powder, which contains 100% <40-μm particles and 80% <5-μm particles.

102 Bordeaux mixture

Solubility Insoluble in water and in organic solvents. Dissolves in ammonium hydroxide, forming a cuprammonium complex. **Stability** No observed deterioration in packs stored in cool, dry places for periods up to 2 years. Chemically not very reactive, but undergoes change if reacted with strong alkalis or acids. When heated, decomposes to black cupric oxide.

COMMERCIALISATION: History The mixture introduced by A. Millardet (*J. Agric. Prat. (Paris)*, 1885, **49**, 513); it may be used as a tank-mix or as pre-formed formulations. Burgundy mixture, introduced by E. Masson (*ibid.*, 1887, **51**, 814), is an analogous product produced from copper sulfate and sodium carbonate. **Manufacturers** Ingenieria Industrial; Isagro; Sulcosa; Tomono.

APPLICATIONS: Biochemistry Copper-II-ion (Cu^{++}) is taken up by the spores during germination and accumulates until a sufficiently high concentration is achieved to kill the spore cell; the activity is limited to the prevention of spore germination. **Mode of action** Foliar fungicide with preventative action. Deposits must be on the crop before fungal spores begin to germinate. **Uses** Bordeaux mixture is used as a protective fungicide for foliage applications, the freshly prepared precipitate having a high tenacity. Its use is limited to crop plants at stages of growth when its phytotoxicity is low. Major uses include the control of *Phytophthora infestans* on potatoes, at 4–6 kg/ha, and *Venturia inaequalis* on apples, *Plasmopara viticola* on grapes, *Sphaceloma perseae* on avocado, at 0.6–0.8 kg/100 l; also *Pseudoperonospora humuli* on hops. Also acts as an insect repellent.

Phytotoxicity Plum and peach foliage may be injured, especially at low temperatures.

Formulation types SC; WP. **Compatibility** Incompatible with alkali-sensitive pesticides such as organophosphorus compounds and carbamates, and with strongly alkaline pesticides, such as lime sulfur. **Selected products** 'Bordocop' (Ingenieria Industrial); 'Flo-Bordo' (Agrichem Manufacturing); 'Poltiglia' (Isagro); 'Z-Bordeaux' (Syngenta Japan).

ANALYSIS: Product analysis is by digestion with sulfuric acid and determination of the copper content by electrolytic, volumetric, gravimetric, colorimetric or atomic absorption spectroscopic methods (*AOAC Methods*, 17th Ed., 920.27–920.30, 922.05, 925.03; *CIPAC Handbook*, 1970, **1**, 226).

Residues determined by digestion with sulfuric acid and perchloric acid, and colorimetry of a complex (*AOAC Methods*, 14th Ed., 25.066–25.071).

MAMMALIAN TOXICOLOGY: Oral Acute oral LD_{50} for rats >4000 mg/kg (WP formulation).

ECOTOXICOLOGY: Fish Toxic to fish. **Bees** Not toxic to bees.

ENVIRONMENTAL FATE: Animals Copper is an essential element and is under homeostatic control in mammals.

ANALYSIS: Product analysis by glc with FID or by hplc (A. A. Carlstrom & J. B. Leary, *Anal. Methods Pestic. Plant Growth Regul.*, 1978, **10**, 173). **Residues** determined by glc with FPD or ECD (*idem, ibid.*; *Pestic. Anal. Man.*, 1979, **1**, 201-1; R. Mestres et al., *Trav. Soc. Pharm. Montpellier*, 1979, **39**, 323; A. Ambrus et al., *J. Assoc. Off. Anal. Chem.*, 1981, **64**, 733; M. A. Luke et al., *ibid.*, p. 1187).

MAMMALIAN TOXICOLOGY: Reviews FAO/WHO 44 (see part 2 of the Bibliography).

IARC ref. 53; class 2A **Oral** Acute oral LD₅₀ for rats 5000–6200 mg a.i./kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >15 400 mg/kg. Corrosive to eyes; mild skin irritant (rabbits). May cause allergic skin reactions in some people. **Inhalation** LC₅₀ for male rats >0.72, female rats 0.87 mg/l (tech.). Dust may cause respiratory irritation. **NOEL** In 2 y feeding trials, no ill-effects observed in rats receiving 500 mg/kg diet and in dogs receiving 10 mg/kg daily. **ADI** (JMPR) Temporary ADI withdrawn [1985]. **Other** Carcinogenic in both rats and mice. **Toxicity class** WHO (a.i.) Ia; EPA (formulation) IV **EC classification** R45| R43| N; R50, R53 **PIC** Yes

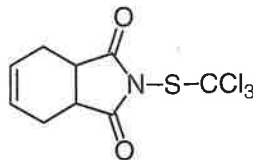
ECOTOXICOLOGY: **Birds** Dietary LC₅₀ (10 d) for pheasants >23 070, mallard ducks >101 700 mg/kg diet. **Fish** LC₅₀ (96 h) for rainbow trout 0.5, goldfish 3.0, bluegill sunfish 0.15 mg/l. **Daphnia** LC₅₀ (96 h) 3.34 ppm. **Other aquatic spp.** Moderately to very highly toxic to freshwater invertebrates. **Bees** Not toxic to bees.

ENVIRONMENTAL FATE: **Animals** In mammals, following oral administration, captanfol is hydrolysed to tetrahydrophthalimide (THPI) and dichloroacetic acid. THPI is degraded to tetrahydrophthalimide acid and further to phthalic acid and ammonia. **Plants** In plants, metabolism is the same as in animals.

114 captan

Fungicide

FRAC M4; multi-site: phthalimide



NOMENCLATURE: **Common name** captan (BSI, E-ISO, JMAF); captane ((m) F-ISO); captab (Republic of South Africa)

IUPAC name N-(trichloromethylthio)cyclohex-4-ene-1,2-dicarboximide

Chemical Abstracts name 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-1H-isoindeole-1,3(2H)-dione

CAS RN [133-06-2] **EC no.** 205-087-0 **Development codes** SR 406

Official codes ENT 26 538

PHYSICAL CHEMISTRY: **Composition** Tech. is 90–95% pure. **Mol. wt.** 300.6

M.f. C₉H₈Cl₃NO₂S **Form** Colourless crystals; (tech. is a colourless to beige amorphous solid, with a pungent odour). **M.p.** 178°C; (tech., 175–178°C) **V.p.** <1.3 mPa (25°C)

K_{ow} logP = 2.8 (25°C) **S.g./density** 1.74 (26°C) **Solubility** In water 3.3 mg/l (25°C). In xylene 20,

captan 133

chloroform 70, acetone 21, cyclohexanone 23, dioxane 47, benzene 21, toluene 6.9, isopropanol 1.7, ethanol 2.9, diethyl ether 2.5 (all in g/kg, 26°C). Insoluble in petroleum oils.

Stability Hydrolysed slowly at neutral pH, rapidly in alkali. Thermal DT₅₀ >4 y (80°C), 14.2 d (120°C).

COMMERCIALISATION: History Fungicide reported by A. R. Kittleston (*Science*, 1952, **115**, 84). Introduced by Standard Oil Development Co., later by Chevron Chemical Co.

Patents US 2553770; US 2553771; US 2553776 **Manufacturers** Arvesta; Crystal; Drexel; Makhteshim-Agan; Rallis; Sharda.

APPLICATIONS: Biochemistry Non-specific thiol reactant, inhibiting respiration.

Mode of action Fungicide with protective and curative action. **Uses** Control of a wide range of fungal diseases, e.g. scab, black rot, botryosphaeria rot, bitter rot, bull's eye rot, botrytis rot of pome fruit; shot-hole of stone fruit; peach leaf curl; brown rots of cherries, apricots, peaches, plums, and citrus fruit; downy mildew and black rot of vines; early and late blights of potatoes and tomatoes; *Alternaria* blight and leaf spot of carrots; anthracnose and downy mildew of cucurbits; leaf spot diseases of ornamentals; anthracnose and leaf spot diseases of tomatoes; brown patch on turf; *Botrytis* spp. on many crops; etc. Used on a large number of other crops. Applied at 2–4.5 lb/a. Used as a seed treatment or root dip for control of *Pythium*, *Phoma*, *Rhizoctonia* spp., etc. on maize, ornamentals, vegetables, oilseed rape, and other crops. **Phytotoxicity** Non-phytotoxic if used as directed, but some varieties of apple (e.g. Red Delicious, Winesap) and pear (e.g. D'Anjou, Bosc) may be injured, as also may lettuce seeds and, at higher dosages, celery and tomato seeds.

Formulation types DP; DS; SC; WG; WP; WS. **Compatibility** Incompatible with alkaline materials, oil sprays, TEPP, and emulsifiable concentrate formulations of parathion.

Selected products 'Capone 480' (Ingeniería Industrial); 'Captaf' (Rallis); 'Captec' (Micro Flo); 'Criptan' (Vapco); 'Dhanutan' (Dhanuka); 'Lucaptan' (Lucava); 'Merpan' (Makhteshim-Agan); **mixtures** 'Bayleton CA' (+ triadimefon) (Bayer CropScience); 'Rondo' (+ pyrifenoxy) (Syngenta).

ANALYSIS: Product analysis by glc (*CIPAC Handbook*, 1985, **1C**, 2015), by hplc (*AOAC Methods*, 17th Ed., 980.06; *CIPAC Handbook*, 1985, **1C**, 2013), by i.r. spectrometry or by total chlorine content after alkaline hydrolysis (*ibid.*, 1970, **1**, 171). **Residues** determined by glc (A. Ambrus et al., *J. Assoc. Off. Anal. Chem.*, 1981, **64**, 733; M. A. Luke et al., *ibid.*, p. 1187; J. N. Ospenson, *Anal. Methods Pestic. Plant Growth Regul. Food Addit.*, 1964, **3**, 7; *Anal. Methods Pestic. Plant Growth Regul.*, 1972, **6**, 546) or by spectrophotometry of a derivative (*AOAC Methods*, 17th Ed., 957.14*).

MAMMALIAN TOXICOLOGY: Reviews FAO/WHO 74, 76, 89 (see part 2 of the Bibliography).

IARC ref. 30; **class** 3 **Oral** Acute oral LD₅₀ for rats 9000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >4500 mg/kg. Corrosive to eyes; mild skin irritant (rabbits).

Inhalation LC₅₀ for rats 0.668 mg/l (tech.). Dust may cause respiratory irritation. **NOEL** (2 y) for rats 2000, dogs 4000 mg/kg diet. No carcinogenic, teratogenic, or mutagenic effects observed.

ADI (JMPR) 0.1 mg/kg b.w. [1995, 2000]. **Toxicity class** WHO (a.i.) U; EPA (formulation) IV **EC classification** R40| T; R23| Xi; R41| R43| N; R50

ECOTOXICOLOGY: Birds Acute oral LD₅₀ for mallard ducks and pheasants >5000, bobwhite quail 2000–4000 mg/kg. Not toxic to starlings or red-winged blackbirds at 100 mg/kg.

Fish LC₅₀ (96 h) for bluegill sunfish 0.072, harlequin fish 0.3, brook trout 0.034 mg/l.

Daphnia LC₅₀ (48 h) 7–10 mg/l. **Other aquatic spp.** Moderately toxic to aquatic invertebrates.

Bees LD₅₀ (oral) 91 µg/bee; (contact) 788 µg/bee.

ENVIRONMENTAL FATE: Animals In mammals, the three chlorine atoms are cleaved under the influence of cellular sulfhydryl compounds. Trithiocarbamate, thiophosgene, and tetrahydrophthalimide are formed (R. G. Owens, *Ann. New York Acad. Sci.*, 1969, **160**, 114–132).

Soil/Environment Soil K_d 3–8 (pH 4.5–7.2, o.m. 2.2–6.7%); DT₅₀ c. 1 d (25°C, pH 7.2, o.m. 1.2%).

acaricide and detachant. **Uses** Used in dips or as a spray, it controls all Acarina species, including strains resistant to organochlorine, organophosphorus and carbamate ixodicides, at concentrations >0.1 g/l. **Formulation types** EC.

ANALYSIS: **Product** analysis by glc. **Residues** determined by glc using FPD or PND. Particulars available from Syngenta.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats 725 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >3100 mg/kg. Slight irritant to skin and eyes of rabbits.

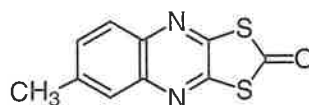
Inhalation LC₅₀ (4 h) for rats >2800 mg/m³ air. **NOEL** (2 y) for rats 10, mice 100 ppm; not oncogenic, not carcinogenic. **Toxicity class** WHO (a.i.) II (company classification)

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for Japanese quail 1212, Pekin ducklings 540 mg/kg.

Fish LC₅₀ (96 h) for rainbow trout 12, carp 32 mg/l.

ENVIRONMENTAL FATE: **Soil/Environment** DT₅₀ <14 d (aerobic soils).

126 chinomethionat *Fungicide, acaricide*



NOMENCLATURE: **Common name** chinomethionat (E-ISO); chinométhionate ((m) F-ISO); quinomethionate (BSI); oxythioquinox (Australia, ESA); quinoxalines (JMAF); no name (USA)
IUPAC name S,S-(6-methylquinoxaline-2,3-diyl) dithiocarbonate;

6-methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one

Chemical Abstracts name 6-methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one

CAS RN [2439-01-2] **EC no.** 219-455-3 **Development codes** Bayer 36 205; Bayer SAS 2074

Official codes ENT 25 606

PHYSICAL CHEMISTRY: **Mol. wt.** 234.3 **M.f.** C₁₀H₆N₂OS₂ **Form** Yellow crystals. **M.p.** 170°C
V.p. 0.026 mPa (20°C) **K_{ow}** logP = 3.78 (20°C) **Henry** 6.09 × 10⁻³ Pa m³ mol⁻¹ (calc.)

S.g./density 1.556 (20°C) **Solubility** In water 1 mg/l (20°C). In toluene 25, dichloromethane 40, hexane 1.8, isopropanol 0.9, cyclohexanone 18, dimethylformamide 10, petroleum oils 4 (all in g/l, 20°C). Soluble in hot benzene and dioxane. **Stability** Relatively stable under normal conditions. Hydrolysed in alkaline media; DT₅₀ (22°C) 10 d (pH 4), 80 h (pH 7), 225 min (pH 9).

COMMERCIALISATION: **History** Acaricide and fungicide reported by K. Sasse (*Hoefchen-Briefe* (Engl. Ed.), 1960, **13**, 197; K. Sasse et al., *Angew. Chem.*, 1960, **72**, 973). Introduced by Bayer AG.
Patents DE 1100372; BE 580478 **Manufacturers** Bayer CropScience.

APPLICATIONS: **Mode of action** Selective non-systemic contact fungicide with protective and eradicant action. **Uses** Control of powdery mildews and spider mites on fruit (including citrus), ornamentals, cucurbits, cotton, coffee, tea, tobacco, walnuts, vegetables, and glasshouse crops; American gooseberry mildew on gooseberries and currants. **Phytotoxicity** Phytotoxic to certain varieties of apple, pear, currant, rose, and ornamentals. **Formulation types** DP; FU; SC; WP.
Compatibility Incompatible with mineral oils (phytotoxicity may result), and with formulations based on thiram. **Selected products** 'Morestan' (Bayer CropScience).

chinomethionat 149

ANALYSIS: Product analysis by hplc (CIPAC Handbook, 1985, 1C, 2019; AOAC Methods, 17th Ed., 986.08) or by u.v. spectrometry (details available from Bayer CropScience). **Residues** determined by glc (Pestic. Anal. Man., 1979, I, 201-I, II; Man. Pestic. Residue Anal., 1987, I, S13; A. Ambrus et al., J. Assoc. Off. Anal. Chem., 1981, 64, 733; R. T. Krause & E. M. August, *ibid.*, 1983, 66, 1018), or by colorimetry after conversion to a derivative (H. Tietz et al., *ibid.*, 1962, 15, 166; C. A. Anderson, Anal. Methods Pestic. Plant Growth Regul. Food Addit., 1967, 5, 277). Methods for the determination of residues are also available from Bayer CropScience.

MAMMALIAN TOXICOLOGY: Reviews FAO/WHO 50, 52 (see part 2 of the Bibliography).

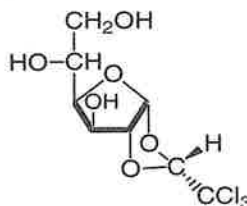
Oral Acute oral LD₅₀ for male rats 2541, female rats 1095 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >5000 mg/kg. Slightly irritating to skin; severely irritating to eyes (rabbits). **Inhalation** LC₅₀ (4 h) for male rats >4.7, female rats 2.2 mg/l (dust). **NOEL** (2 y) for rats 40, male mice 270, female mice <90 mg/kg diet; (1 y) for dogs 25 mg/kg diet. **ADI** (JMPR) 0.006 mg/kg b.w. [1987]. **Toxicity class** WHO (a.i.) III; EPA (formulation) III **EC classification** R62|Xn; R20/21/22, R48/22|Xi; R36| R43| N; R50, R53

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail 196 mg/kg. Dietary LC₅₀ (5 d) for bobwhite quail 2409, mallard ducks >5000 mg/kg diet. **Fish** LC₅₀ (96 h) for bluegill sunfish 0.0334, rainbow trout 0.131, golden orfe 0.24 mg/l. **Daphnia** LC₅₀ (48 h) 0.12 mg/l. **Algae** E_r-C₅₀ (96 h) for *Scenedesmus* 0.14 mg/l. **Bees** Not toxic to bees; LD₅₀ >100 µg/bee. **Worms** LC₅₀ (14 d) >1000 mg/kg.

ENVIRONMENTAL FATE: **Animals** In rats, following oral administration, chinomethionat is rapidly metabolised, and c. 90% is eliminated within 3 days in the faeces and urine. The main metabolite is chinomethionat acid (dimethylmercaptoquinoxaline-6-carboxylic acid), which also occurs in the conjugated form. **Plants** After application to fruit, no penetration of the a.i. or metabolites in the fruit pulp was observed. The only metabolite detected was dihydromethylquinoxalinedithiol. **Soil/Environment** K_{oc} 45–90 (3 soil types from sandy loam to high organic matter). DT₅₀ in standard soil land 2 1–3 d.

127 chloralose

Rodenticide



NOMENCLATURE: **Common name** chloralose (BSI, E-ISO, F-ISO); glucochloralose (BSI, E-ISO); glucochloral (F-ISO); are all accepted in lieu

IUPAC name (R)-1,2-O-(2,2,2-trichloroethylidene)-α-D-glucofuranose

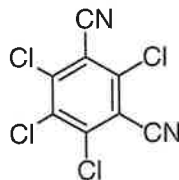
Chemical Abstracts name (R)-1,2-O-(2,2,2-trichloroethylidene)-α-D-glucofuranose

Other names alphachloralose **CAS RN** [15879–93–3], formerly [39598–39–5] or [14798–36–8]; [16376–36–6] beta-form **EC no.** 240–016–7

PHYSICAL CHEMISTRY: **Composition** Chloralose also exists in a beta-form. **Mol. wt.** 309.5

150 chloralose

FRAC M5; multi-site: chloronitrile



NOMENCLATURE: Common name chlorothalonil (BSI, E-ISO, (m) F-ISO, ANSI); TPN (JMAF)
IUPAC name tetrachloroisophthalonitrile
Chemical Abstracts name 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile
CAS RN [1897-45-6] **EC no.** 217-588-1 **Development codes** DS-2787 (Diamond Shamrock)

PHYSICAL CHEMISTRY: **Composition** Tech. is c. 97%. **Mol. wt.** 265.9 **M.f.** C₈Cl₄N₂
Form Colourless, odourless crystals; (tech. has a slightly pungent odour). **M.p.** 252.1 °C
B.p. 350 °C/760 mmHg **V.p.** 0.076 mPa (25 °C) **K_{ow} logP** = 2.92 (25 °C) **Henry** 2.50 × 10⁻² Pa m³ mol⁻¹ (25 °C) **S.g./density** 2.0 (20 °C) **Solubility** In water 0.81 mg/l (25 °C). In xylene 80, cyclohexanone, dimethylformamide 30, acetone, dimethyl sulfoxide 20; kerosene <10 (all in g/kg, 25 °C). **Stability** Thermally stable at ambient temperatures. Stable to u.v. light in aqueous media and in crystalline state. Stable in acidic and moderately alkaline aqueous solutions; slow hydrolysis at pH >9.

COMMERCIALISATION: **History** Fungicide reported by N. J. Turner et al. (*Contrib. Boyce Thompson Inst.*, 1964, **22**, 303). Introduced by the Diamond Alkali Co. (later ISK Biosciences Corp.) and sold to Zeneca Agrochemicals (now Syngenta AG) in 1997. **Patents** US 3290353; US 3331735
Manufacturers Agrochem; GB Biosciences; Gharda; Gilmore; Isagro; SDS Biotech KK; Sundat.

APPLICATIONS: **Biochemistry** Conjugation with, and depletion of, thiols (particularly glutathione) from germinating fungal cells, leading to disruption of glycolysis and energy production, fungistasis and fungicidal action. **Mode of action** Non-systemic foliar fungicide with protective action.
Uses Control of many fungal diseases in a wide range of crops, including pome fruit, stone fruit, citrus fruit, bush and cane fruit, cranberries, strawberries, pawpaws, bananas, mangoes, coconut palms, oil palms, rubber, pepper, vines, hops, vegetables, cucurbits, tobacco, coffee, tea, rice, soya beans, peanuts, potatoes, sugar beet, cotton, maize, ornamentals, mushrooms, and turf. Application rates for food crops are 1–2.5 kg/ha. **Phytotoxicity** Russetting is possible with flowering ornamentals, apples, and grapes. Some varieties of flowering ornamentals may be injured. *Pittosporum* foliage is sensitive. Phytotoxicity may be increased with oils or oil-containing substances. **Formulation types** SC; WG; WP; Fogging concentrate. **Compatibility** Not compatible with oils. **Selected products** 'Bravo' (Syngenta); 'Daconil' (Syngenta, SDS Biotech KK); 'Banko' (Calliope); 'Bombardier' (Unicrop); 'Chloronil' (Vapco); 'Clortosip' (Sipcam); 'Corrib' (Barclay); 'Equus' (Nations Ag); 'Fungiless' (Sanonda); 'Gilonil' (Gilmore); 'Mycoguard' (Chiltern, Gharda); 'Oranil' (Cequisa); 'Talonil' (Ingeniería Industrial); 'Teren' (Efthymiadis); 'Visclor' (Vischim).

ANALYSIS: **Product** analysis by glc (AOAC Methods, 17th Ed., 999.04; D. L. Ballee et al., *Anal. Methods Pestic. Plant Growth Regul.*, 1976, **8**, 263). **Residues** determined by gc-ms; details available from Syngenta. In **drinking water** by glc with ECD (AOAC Methods, 17th Ed., 990.06). Details available from Syngenta.

MAMMALIAN TOXICOLOGY: **Reviews** CAG (see part 2 of Bibliography). **IARC ref.** 30; 73;

class 2B Oral Acute oral LD₅₀ for rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for albino rabbits >5000 mg/kg. Severe eye irritant; mild skin irritant (rabbits). Evidence in humans of contact dermatitis with repeated exposure. **Inhalation** LC₅₀ (1 h) for rats 0.52 mg/l air; (4 h) for rats 0.10 mg/l air. **NOEL** Chronic administration of chlorothalonil has been associated with renal hyperplasia and hyperkeratosis of the forestomach in the kidney and forestomach of rats and male mice. These pre-neoplastic lesions precede subsequent tumour development in the rodent kidney and forestomach. The mode of action has been demonstrated to be epigenetic, with a NOEL of 1.8 in rats and 1.6 in mice. In dogs, the pattern of toxicity is different from that in rodents, with no evidence of toxicity in the kidney or forestomach, and a NOEL of at least 3 mg/kg b.w. (JMPR 1994). **ADI** (JMPR) 0.03 mg/kg [1994]; (EPA) 0.02 mg/kg [RED 1998]. **Toxicity class** WHO (a.i.) U; EPA (formulation) II ('Bravo' SC) **EC classification** R40| N; R50, R53

ECOTOXICOLOGY: Birds Acute oral LD₅₀ for mallard ducks >4640 mg/kg. Dietary LC₅₀ (8 d) for mallard ducks and bobwhite quail >10 000 mg/kg diet. **Fish** LC₅₀ (96 h) for rainbow trout 47, bluegill sunfish 59, channel catfish 43 µg/l. **Daphnia** LC₅₀ (48 h) 70 µg/l. **Algae** EC₅₀ (120 h) for *Selenastrum capricornutum* 210 µg/l; EC₅₀ (72 h) for *Navicula pelliculosa* 5.1 µg/l.

Other aquatic spp. LC₅₀ (48 h) for *Crangonyx pseudogracilis* 64, *Chironomus riparius* 110, *Cloeon dipterum* 600 µg/l; LC₅₀ (24 h) for *Brachionus calyciflorus* 24 µg/l. **Bees** LD₅₀ for honeybees (oral) >63 µg/bee; (contact) >101 µg/bee. **Worms** LC₅₀ (14 d) >404 mg/kg.

Other beneficial spp. LR₅₀ (7 d) for *Typhlodromus pyri* >18.75 kg/ha; LR₅₀ (48 h) for *Aphidius rhopalosiphi* >18.75 kg/ha.

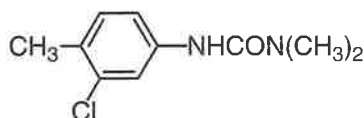
ENVIRONMENTAL FATE: EHC 183 (WHO, 1996) Animals Chlorothalonil is not well absorbed following oral dosing. It reacts with glutathione in the gut lumen, or immediately on absorption into the body, to give mono-, di- or tri- glutathione conjugates. These may be excreted through urine or faeces, or subject to further metabolism resulting in thiol or mercapturic acid derivatives. Excretion of these in urine is believed to be significantly greater in rats than in dogs or primates. In ruminants, the major identified metabolite is the 4-hydroxy derivative; no parent material is found.

Plants In plants, the majority of residues remain as parent compound; 4-hydroxy-2,5,6-trichloro- isophthalonitrile is found as a metabolite to a limited extent. **Soil/Environment** K_{oc} 1600 (sand) to 14 000 (silt), indicating low mobility to immobile. In aerobic and anaerobic soil studies, DT₅₀ is 0.3–28 d (20°C). Stable to hydrolysis at pH 5–7; at pH 9 (22°C), DT₅₀ is 38 d. Degradation is faster in biotic aquatic systems; typical DT₅₀ (aerobic) <8 h, (anaerobic) <10 d. A wide variety of metabolites are formed, which are, in turn, degraded further.

143 chlorotoluron

Herbicide

HRAC C₂ WSSA 7; urea



NOMENCLATURE: Common name chlorotoluron (BSI (from 1984), E-ISO, (m) F-ISO); chlortoluron (BSI (before 1984), (m) France, New Zealand)

IUPAC name 3-(3-chloro-*p*-tolyl)-1,1-dimethylurea

Chemical Abstracts name *N'*-(3-chloro-4-methylphenyl)-*N,N*-dimethylurea

170 chlorotoluron

ANALYSIS: Product analysis by iodometric titration (AOAC Methods, 14th Ed., 6.015–6.016; CIPAC Handbook, 1970, 1, 226).

MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats 489 mg/kg (tech.).

Skin and eye Acute percutaneous LD₅₀ for rabbits >3160 mg/kg. Severely irritating and corrosive to eyes; mild skin irritant. **Inhalation** LC₅₀ >2 mg/l air. **Toxicity class** WHO (a.i.) III; EPA (formulation) III

ECOTOXICOLOGY: High concentrations of this type of copper are toxic to aquatic organisms and may cause a significant decrease in populations of aquatic invertebrates, plants, and fish.

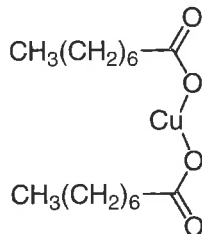
Birds Acute oral LD₅₀ for bobwhite quail 3400, mallard ducks >5000 mg/kg. Dietary LC₅₀ (8 d) for bobwhite quail and mallard ducks >10 000 ppm. **Fish** LC₅₀ (24 h) for rainbow trout 0.08 mg/l; (96 h) for fathead minnows 0.023, bluegill sunfish >180 mg/l. **Daphnia** LC₅₀ 6.5 ppb. **Bees** Non-toxic to honeybees.

ENVIRONMENTAL FATE: **Animals** Copper is an essential element and is under homeostatic control in mammals. **Plants** Plants resist copper accumulation and translocation to stems, leaves or seeds. Most plants growing on soils containing up to 1000 ppm copper showed only slight elevation in copper content, compared to plants grown in normal soils. **Soil/Environment** Copper is a basic chemical element and does not dissipate in the soil. Soluble copper ions in the soil water are rapidly complexed by organic matter, precipitated as hydroxides, or insolubilised as precipitates with sulfides, hydroxides, carbonates, or phosphates.

170 copper octanoate

Fungicide, bactericide, algicide

FRAC M1; multi-site: inorganic



NOMENCLATURE: IUPAC name copper dioctanoate

CAS RN [20543–04–8] Development codes NEU 1140 F (Neudorff)

PHYSICAL CHEMISTRY: Mol. wt. 350.0 M.f. C₁₆H₃₀CuO₄ Form Solid.
S.g./density 1.048 (20°C)

COMMERCIALISATION: History Registered in US in 1997. Patents US 5246716; EP 0580821

APPLICATIONS: Uses Control of powdery mildews (*Erysiphe*, *Sphaerotheca*, *Uncinula*, *Microsphaera*), downy mildews (*Plasmopara*, *Peronospora*, *Bremia*), leaf and fruit spots (*Alternaria*,

copper octanoate 203

Colletotrichum, *Drechslera*, *Erwinia*, *Pseudomonas*, *Septoria*, *Taphrina*, *Xanthomonas*), blights (*Phytophthora*, *Rhizoctonia*), and rusts (*Phragmidium*, *Puccinia*, *Uromyces*). **Phytotoxicity** May cause copper toxicity on some rose varieties. May cause russetting on some apple varieties. **Compatibility** Not compatible with oils. **Selected products** 'NEU1140F Copper Soap' (Neudorff).

ANALYSIS: The copper content is determined by EPA Atomic Absorption Methods 7210 and 3005.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats >2000 mg 'NEU1140F' formulation/kg. **Skin and eye** Acute dermal LD₅₀ for rats >2000 mg 'NEU1140F' formulation/kg. No skin or eye irritation (rabbits). Not a skin sensitiser (guinea pigs). **Inhalation** EC₅₀ for rats >0.38 mg 'NEU1140F' formulation/l. **Toxicity class** EPA (formulation) III

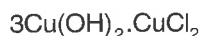
ECOTOXICOLOGY: **Fish** Toxic to fish. **Bees** Not toxic to bees. **Worms** Not toxic to earthworms.

ENVIRONMENTAL FATE: **Soil/Environment** Degrades to free copper and octanoic acid; the latter is expected to degrade further microbially.

171 copper oxychloride

Fungicide

FRAC M1; multi-site: inorganic



NOMENCLATURE: **Common name** copper oxychloride (E-ISO, accepted in lieu of common name); oxychlorure de cuivre (F-ISO)

IUPAC name dicopper chloride trihydroxide (approximate composition); copper oxychloride

Chemical Abstracts name copper chloride oxide hydrate

Other names copper chloride hydroxide **CAS RN** [1332-40-7]; [1332-65-6] defined as copper chloride hydroxide **EC no.** 215-572-9

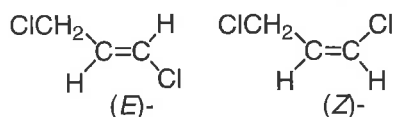
PHYSICAL CHEMISTRY: **Composition** Contains 57% Cu⁺⁺. **Mol. wt.** 427.1 **M.f.** Cl₂Cu₄H₆O₆ **Form** Green to bluish-green powder. **M.p.** decomp. 300°C **V.p.** Negligible at 20°C **Solubility** In water <10⁻⁵ mg/l (pH 7, 20°C). Insoluble in organic solvents. Soluble in dilute acids, forming Cu(II) salts; soluble in ammonium hydroxide, forming a complex ion. **Stability** Very stable in neutral media. Decomposes on heating in alkaline media, with the formation of copper oxides. Decomposes on heating, with the formation of copper oxides and loss of hydrogen chloride.

COMMERCIALISATION: **History** Introduced as a fungicide in the early 1900s.

Manufacturers Aimco; Crystal; Griffin; Hokko; Ingenierfa Industrial; Isagro; Rallis; Sharda; Sulcosa; Syngenta; Tagros.

APPLICATIONS: **Biochemistry** Copper-II ion (Cu⁺⁺) is taken up by the spores during germination and accumulates until a sufficiently high concentration is achieved to kill the spore cell; the activity is limited to the prevention of spore germination. **Mode of action** Foliar fungicide with preventative action. Deposits must be on the crop before fungal spores begin to germinate. **Uses** Control of late blight of potatoes, tomatoes and other vegetables; leaf spot diseases of beet, celery, celeriac, parsley, olives, currants, and gooseberries; downy mildews of vines, hops, spinach, and ornamentals; canker and scab of pome fruit and stone fruit; scab, canker, and melanose of citrus fruit; asparagus

204 copper oxychloride



NOMENCLATURE: **Common name** 1,3-dichloropropene (BSI, E-ISO accepted in lieu of a common name); dichloro-1,3-propene (F-ISO); D-D (JMAF (name also used for mixture with 1,2-dichloropropane))

IUPAC name (E)-1,3-dichloropropene

Chemical Abstracts name 1,3-dichloro-1-propene

CAS RN [542-75-6] (E)- + (Z)- isomers; [10061-02-6] (E)- isomer; [10061-01-5] (Z)- isomer

EC no. 208-826-5 ((E)- + (Z)- isomers); 233-195-8 ((Z)- isomer)

PHYSICAL CHEMISTRY: **Composition** Tech. product is 97–98% pure. It is a mixture of approximately equal quantities of (E)- and (Z)- isomers. **Mol. wt.** 111.0 **M.f.** C₃H₄Cl₂
Form Colourless-to-amber liquid, with a sweet penetrating odour (tech.). **M.p.** <–50°C
B.p. 108°C; (Z)- isomer 104.3°C; (E)- isomer 112°C **V.p.** 3.7 kPa; (E)- isomer 2.3 kPa; (Z)- isomer 3.5 kPa (all at 20°C) **K_{ow}** logP = 1.82 (20°C); (E)- isomer 2.03; (Z)- isomer 2.06 (both 25°C)
S.g./density 1.214 (20°C); (E)- isomer 1.224; (Z)- isomer 1.217 **Solubility** In water 2 g/l (20°C); (E)- isomer 2.32, (Z)- isomer 2.18 (both in g/l, 25°C). Miscible with hydrocarbons, halogenated solvents, esters, and ketones. **Stability** Stable under normal conditions. DT₅₀ 11.3 d (pH 5–9, 20°C). **F.p.** 25°C (Abel closed cup)

COMMERCIALISATION: **History** Properties as a soil fumigant reported by Dow Chemical Co. (now Dow AgroSciences), who introduced it (*Down Earth*, 1956, 12(2), 7). **Manufacturers** Dow AgroSciences.

APPLICATIONS: **Mode of action** Soil fumigant nematicide. Both isomers are active; the (Z)- isomer is the more effective to nematodes (C. R. Youngson & C. A. I. Goring, *Plant Dis. Rep.*, 1970, 54, 196). **Uses** Pre-planting control of most species of nematode in deciduous fruit and nuts, citrus fruit, berry fruit, vines, strawberries, hops, field crops, vegetables, tobacco, beet, pineapples, peanuts, ornamental and flower crops, tree nurseries, etc. Also has secondary insecticidal (soil insects) and fungicidal activity, and, by controlling nematode virus vectors, control is obtained of virus diseases of strawberries, raspberries, tomatoes, hops, etc. Applied at 60–350 lb/a.

Phytotoxicity Can be phytotoxic if crops are planted too soon after application.

Formulation types Liquid. **Selected products** 'Telone II' (Dow AgroSciences); 'D-D' (BASF); 'Nematrap' (BASF).

ANALYSIS: **Product** analysis by glc: details from Dow AgroSciences and BASF.

Residues determined by glc (M. V. McKenry & I. J. Thomason, *Hilgardia*, 1974, 42, 393; T. R. Roberts & G. Stoydin, *Pestic. Sci.*, 1976, 7, 325). Methods reviewed by J. L. Daft in *Comp. Analyt. Profiles*, Chapter 11.

MAMMALIAN TOXICOLOGY: **IARC ref.** 41; Suppl. 7; 71; **class** 2B **Oral** Acute oral LD₅₀ for rats 150 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats 1200 mg/kg. Severely irritating to skin, eyes and mucous membranes. Prolonged contact with skin can cause severe burns.

Inhalation LC₅₀ (4 h) for rats 2.70–3.07 mg/l air. See also NOEL data. **NOEL** In 90 d inhalation studies, NOEL for rats and mice 0.05 mg/l air. In 2 y inhalation studies, NOEL for rats 0.099, mice 0.025 mg/l air. Not embryotoxic or teratogenic in rats and rabbits in inhalation studies at 0.59 mg/l. In 2-generation inhalation studies, NOEL on reproduction in rats 0.45 mg/l air.

Toxicity class WHO (a.i.) FM; EPA (formulation) III **EC classification** R10| T; R25| Xn; R20/21| Xi; R36/37/38| R43| N; R50, R53 (for both (E)- + (Z)- isomers, and (Z)- isomer)

ECOTOXICOLOGY: **Birds** LD₅₀ for bobwhite quail 152 mg/kg. Dietary LC₅₀ (5 d) for mallard ducks and bobwhite quail >10 000 mg/kg diet. **Fish** LC₅₀ (96 h) for rainbow trout 3.9, bluegill sunfish 7.1 mg/l. **Daphnia** LC₅₀ (48 h) 6.2 mg/l. **Algae** Slightly toxic.

Other aquatic spp. Moderate acute toxicity. **Bees** LD₅₀ (90 h) 6.6 µg/bee. **Worms** Initially toxic to earthworms; not persistent, therefore re-colonisation is very quick.

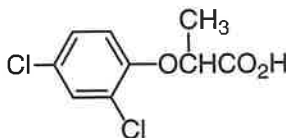
ENVIRONMENTAL FATE: EHC 146 (WHO, 1993). **Animals** Excretion in rats occurred primarily as the mercapturic acid conjugate and its corresponding sulfoxide. **Plants** Metabolism is rapid, progressing through 3-chloroallyl alcohol, 3-chloroacrylic acid and 3-chloro-1-propanol, leading ultimately to normal plant constituents (D. L. Berry et al., *J. Food Safety*, 1980, **4**, 247–255); metabolic DT₅₀ for 1,3-dichloropropene 1.5 h, for 3-chloroallyl alcohol 4.4 h (both calc.).

Soil/Environment Non-persistent in soil, undergoing hydrolysis to the corresponding 3-chloroallyl alcohols (C. E. Castro & N. O. Belser, *J. Agric. Food Chem.*, 1966, **14**, 69; T. R. Roberts & G. Stoydin, *Pestic. Sci.*, 1976, **7**, 325; M. V. McKenry & I. J. Thomason, *Hilgardia*, 1974, **42**, 393). Aerobic lab. DT₅₀ (13 soils) 6–17 d (20°C). Anaerobic DT₅₀ (average) 8.4 d (15°C), 2.4 d (25°C). Hydrolysis DT₅₀ 11 d (pH 5–9, 20°C).

234 dichlorprop

Herbicide

HRAC O WSSA 4; phenoxyacetic acid



NOMENCLATURE: *dichlorprop*

Common name dichlorprop (BSI, E-ISO, (m) F-ISO, WSSA); 2,4-DP* (former exception, USSR)

IUPAC name (R_S)-2-(2,4-dichlorophenoxy)propionic acid

Chemical Abstracts name (±)-2-(2,4-dichlorophenoxy)propanoic acid

Other names 2,4-DP **CAS RN** [7547–66–2] racemic acid; [120–36–5] dichlorprop (unstated stereochemistry) **EC no.** 204–390–5 **Development codes** RD 406 (AgrEvo)

dichlorprop-isooctyl

CAS RN [28631–35–8]

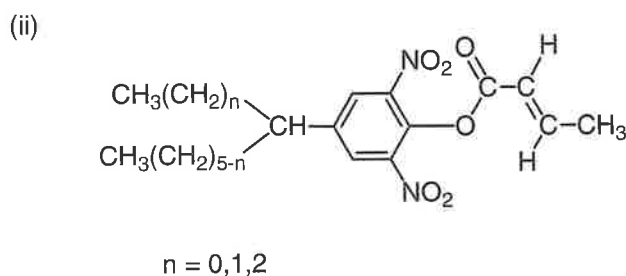
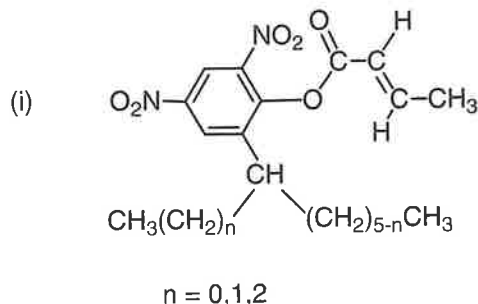
PHYSICAL CHEMISTRY: *dichlorprop*

Composition Commercial dichlorprop is a racemate, only the (+)-isomer (q.v.) being herbicidally active. **Mol. wt.** 235.1 **M.f.** C₉H₈Cl₂O₃ **Form** Colourless crystals; (tech. is a brown powder, with a phenolic odour). **M.p.** 116–117.5°C; (tech., 114°C) **V.p.** <1 × 10⁻² mPa (20°C)

K_{ow} logP = 1.77 (unstated pH) **S.g./density** 1.42 **Solubility** In water 350 mg/l (20°C). In acetone 595, isopropanol 510, benzene 85, toluene 69, xylene 51, kerosene 2.1 (all in g/l, 20°C). Sodium salt: In water 660 g acid equivalent/l (20°C). Diethanolamine salt: In water 740 g acid equivalent/l (20°C). **Stability** The acid is very stable, and forms sparingly-soluble, slightly-active salts with heavy metals. **pKa** 3.00 **F.p.** 204°C (open cup)

dichlorprop 287

FRAC 29, C5

**NOMENCLATURE:** Common name dinocap (BSI, E-ISO, (m) F-ISO); DPC (JMAF);

no name (Republic of South Africa)

IUPAC name 2,6-dinitro-4-octylphenyl crotonates and 2,4-dinitro-6-octylphenyl crotonates in which 'octyl' is a mixture of 1-methylheptyl, 1-ethylhexyl and 1-propylpentyl groups**Chemical Abstracts name** (E)-2-(1-methylheptyl)-4,6-dinitrophenyl 2-butenate**CAS RN** [131-72-6] single compound; [39300-45-3] mixed isomers but unstatedstereochemistry **EC no.** 254-408-0 (for mixed isomers) **Development codes** CR-1693**Official codes** ENT 24 727

PHYSICAL CHEMISTRY: **Composition** Originally thought to be 2-(1-methylheptyl)-4,6-dinitrophenyl crotonate (i, $n=0$). Now known that the commercial material is a mixture comprising 2.0–2.5 parts of 6-octyl isomers (i) to 1.0 part of 4-octyl isomers (ii). See IUPAC definition for specification of 'octyl'. **Mol. wt.** 364.4 **M.f.** $C_{18}H_{24}N_2O_6$ **Form** Dark red viscous liquid, with a pungent odour. **M.p.** -22.5°C **B.p.** $138\text{--}140^\circ\text{C}/0.05\text{ mmHg}$; at ambient pressure, decomp. above 200°C **V.p.** $3.33 \times 10^{-3}\text{ mPa}$ (25°C , vapour pressure balance) **K_{ow}** $\log P = 4.54$ (20°C) **Henry** $1.36 \times 10^{-3}\text{ Pa m}^3\text{ mol}^{-1}$ (calc.) **S.g./density** 1.10 (20°C) **Solubility** In water 0.151 mg/l. 2,4- isomer: in acetone, 1,2-dichloroethane, ethyl acetate, *n*-heptane, methanol and xylene >250 g/l; 2,6- isomer: in acetone, 1,2-dichloroethane, ethyl acetate and xylene >250, *n*-heptane 8.5–10.2, methanol 20.4–25.3 (all in g/l). **Stability** Rapidly decomposed by light. Decomposes > 32°C . Stable in acidic media. Hydrolysis of the ester group occurs in alkaline media. 2-(1-methylheptyl)-4,6-dinitrophenyl crotonate hydrolysed in aqueous methanol; (25°C) DT_{50} 229 d (pH 5), 56 h (pH 7), 17 h (pH 9). **F.p.** 67°C (Pensky-Martens closed cup)

COMMERCIALISATION: **History** Introduced by Rohm & Haas Co. (now Dow AgroSciences).
Patents US 2526660; US 2810767 **Manufacturers** Dow AgroSciences.

APPLICATIONS: **Biochemistry** Uncouples mitochondrial oxidative phosphorylation.

Mode of action Contact fungicide with protective and curative action. Secondary effect as a non-systemic acaricide. **Uses** Primarily sold as a mildewicide for use on *Uncinula necator* in grapes in Europe (at 210 g/ha). Also used to control powdery mildews of various crops, including pome and stone fruit, citrus, cucurbits, vegetables, tobacco, hops and ornamentals. Secondly causes some suppression of phytophagous mites, such as *Panonychus ulmi* and *Hemitarsonemus latus* (citrus silver mite). **Phytotoxicity** Non-phytotoxic, except for glasshouse roses under certain conditions. Phytotoxicity is increased at higher temperatures. **Formulation types** DP; EC; WP.

Compatibility Incompatible with oils and oil-based sprays, and alkaline materials.

Selected products 'Karathane' (Dow AgroSciences); 'Sialite' (Siapa).

ANALYSIS: **Product** analysis by spectrophotometry (R. F. Black *et al.*, *J. Assoc. Off. Anal. Chem.*, 1974, **57**, 653), or by lc; details available from Dow AgroSciences. **Residues** determined by glc (A. Ambrus *et al.*, *ibid.*, 1981, **64**, 733; *Pestic. Anal. Man.*, 1979, **1**, 201-A, 201-G, 201-I; *Man. Pestic. Residue Anal.*, 1987, **1**, S19; *Anal. Methods Residues Pestic.*, 1988, Part II; *Anal. Methods Pestic. Plant Growth Regul.*, 1972, **6**, 568).

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 89 (see part 2 of the Bibliography).

Oral Acute oral LD₅₀ for male rats 990, female rats 1212 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits ≥2000 mg/kg. Irritating to skin and eyes (rabbits). **Inhalation** LC₅₀ (4 h) for rats ≥3 mg/l air. **NOEL** (18 mo) for female mice 2.7 mg/kg b.w. daily, for male mice 14.6 mg/kg b.w. daily; (2 y) for rats 6–8 mg/kg b.w. daily; for dogs 0.4 mg/kg b.w. daily. There were no carcinogenic effects in rodents. Teratogenic effects were produced in 3 species, with the relevant NOAEL in mice being 4 mg/kg b.w. daily. **ADI** (JMPR) 0.008 mg/kg b.w. [2000]. **Toxicity class** WHO (a.i.) III; EPA (formulation) III **EC classification** Xn; R22| Xi; R38 (for mixed isomers)

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail >2150 mg/kg. Dietary LC₅₀ (8 d) for mallard ducks 2204, bobwhite quail 2298 ppm. **Fish** Toxic to fish. LC₅₀ for rainbow trout 13, bluegill 5.3, carp 14, fathead minnows 20 µg/l. **Daphnia** LC₅₀ (48 h) 4.2 µg/l. **Algae** EC₅₀ (72 h) >105 mg/l. **Other aquatic spp.** LC₅₀ for *Chironomus riparius* 390 µg/l. **Bees** Low toxicity to bees; acute LD₅₀ (contact) 29 µg/bee; acute LC₅₀ (oral) 6.5 µg/bee. **Worms** LC₅₀ (14 d) 120 mg/kg. **Other beneficial spp.** Under laboratory conditions, dinocap is harmful to *Aphidius rhopalosiphii* and *Typhlodromus pyri*. However, under field conditions, effects are minimised due to rapid degradation. Dinocap has no adverse effects on predatory mites under field conditions when used to label recommendations (M. Miles & E. Green, *Proc. 2002 Br. Crop Prot. Conf. - Pests Dis.*, 297–302).

ENVIRONMENTAL FATE: Dinocap is readily degraded in plants, animals and the environment to give 2,4- and 2,6- dinitrophenol (DNOP). Dinocap and its residues have no significant leaching potential and pose no threat to groundwater. **Animals** In rats, following oral administration, dinocap is almost entirely eliminated rapidly in the urine and faeces. In dairy cows, dinocap and its metabolites are excreted almost completely in the faeces, with only a small amount in the urine. The nitro groups are enzymically reduced to amino groups, and ester hydrolysis also takes place, to give DNOP. **Plants** Metabolism follows the same course as in animals. **Soil/Environment Soil:** DT₅₀ (lab., aerobic, 20°C) 4–24 d; DT₉₀ 13.5–113 d. DT₅₀ (lab., anaerobic, 20°C) 8 d. No significant soil photolysis. The major metabolite is DNOP, formed by ester hydrolysis, with subsequent microbial degradation to CO₂. K_{oc} 2889–310200, depending on soil type; dinocap and its residues have no leaching potential. **Water:** DT₅₀ (sterile, dark, 20°C) >1 y (pH 4), 16–30 d (pH 7), 3.6–9 d (pH 9). Photolysis in water is more rapid; DT₅₀ <1 d (25°C, pH 4). In dark water/sediment systems, dinocap rapidly dissipates from water to sediment, DT₅₀ (lab.) <7 d, and is readily degraded. In

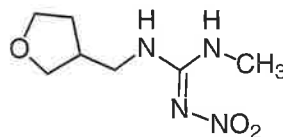
dinocap 335

aquatic systems, the major metabolite is DNOP. **Air:** No significant volatile losses are expected following application. Any small amounts present in air are estimated to degrade with atmospheric DT₅₀ 1.9 h.

271 dinotefuran

Insecticide

IRAC 4A; neonicotinoid



NOMENCLATURE: Common name dinotefuran (BSI, pa ISO)

IUPAC name (RS)-1-methyl-2-nitro-3-(tetrahydro-3-furylmethyl)guanidine

Chemical Abstracts name N-methyl-N'-nitro-N''-[(tetrahydro-3-furanyl)methyl]guanidine

CAS RN [165252-70-0] **Development codes** MTI-446 (Mitsui)

PHYSICAL CHEMISTRY: Mol. wt. 202.2 M.f. C₇H₁₄N₄O₃ M.p. 94.5–101.5 °C

K_{ow} logP = -0.644 (pH 7) **S.g./density** 1.33 **Solubility** In purified water 54.3 ± 1.3 g/l (20 °C).

pKa No dissociation in range pH 1.4 to 12.3

COMMERCIALISATION: **History** Reported by K. Kodaka et al. (*Proc. Br. Crop Prot. Conf. - Pests Dis.*, 1998, 1, 21). Under development by Mitsui Chemicals Inc. **Patents** EP 0649845

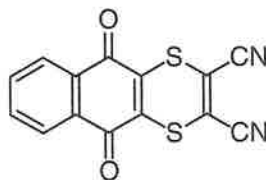
Manufacturers Mitsui.

APPLICATIONS: **Biochemistry** Agonist of the nicotinic acetylcholine receptor, affecting the synapses in the insect central nervous system. **Mode of action** Active by ingestion and by contact; also exhibits root-systemic activity. **Uses** Controls a range of hemipterous and other pests, at 100–200 g/ha. **Selected products** 'Starkle' (Mitsui).

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for male rats 2804, female rats 2000, male mice 2450, female mice 2275 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for male and female rats >2000 mg/kg. Not a skin sensitiser (guinea pigs).

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for mallard ducks 1000, Japanese quail >2000 mg/kg. **Fish** LC₅₀ (96 h) for carp >1000 ppm; (48 h) for rainbow trout >40 ppm. **Daphnia** (48 h) 1000 ppm **Other aquatic spp.** LC₅₀ (48 h) for crayfish 5–10 ppm.

FRAC M9; multi-site: quinone



NOMENCLATURE: **Common name** dithianon (BSI, E-ISO, (m) F-ISO, JMAF); no name (Italy)
IUPAC name 5,10-dihydro-5,10-dioxonaphtho[2,3-b]-1,4-dithiine-2,3-dicarbonitrile
Chemical Abstracts name 5,10-dihydro-5,10-dioxonaphtho[2,3-b]-1,4-dithi-in-2,3-dicarbonitrile
CAS RN [3347-22-6] **EC no.** 222-098-6 **Development codes** IT-931 (E. Merck); MV 119A; CME107 (Celamerck); SAG 107; CL 37114 (Cyanamid); BAS 216F (BASF)

PHYSICAL CHEMISTRY: **Mol. wt.** 296.3 **M.f.** C₁₄H₄N₂O₂S₂ **Form** Dark brown crystals, with a coppery lustre; (tech., lighter brown). **M.p.** 225 °C; (tech., c. 217 °C) **V.p.** 2.7 × 10⁻⁶ mPa (25 °C) **K_{ow} logP** = 3.2 **Henry** 5.71 × 10⁻⁶ Pa m³ mol⁻¹ (calc.) **S.g./density** 1576 kg/m³ (20 °C) **Solubility** In water 0.14 mg/l (pH 7, 20 °C). In chloroform 12, acetone 10, benzene 8 (all in g/l, 20 °C). Sparingly soluble in methanol and dichloromethane. **Stability** Decomposed by alkaline media, by concentrated acids, and by prolonged heating; DT₅₀ 12.2 h (pH 7, 25 °C). Stable up to 80 °C. Aqueous solution (0.1 mg/l) exposed to artificial sunlight had DT₅₀ 19 h. **F.p.** Ignition temperature >300 °C

COMMERCIALISATION: **History** Fungicide reported by J. Berker et al. (*Proc. Br. Insectic. Fungic. Conf.*, 2nd, 1963, p. 351). Introduced by E. Merck and later by Shell Agrar GmbH (now BASF AG). **Patents** GB 857383 **Manufacturers** BASF; Sundat.

APPLICATIONS: **Biochemistry** Affects a range of fungal enzymes by reacting with thiol groups and interfering with cellular respiration. Multi-site mode of action. **Mode of action** Foliar fungicide with protective and, to some extent, curative action. **Uses** Control of many foliar diseases (but not powdery mildews), including scab on pome fruit; *Stigmata carpophila*, *Coccomyces hiemalis* and scab on cherries; *Monilia* spp., rust and leaf curl on peaches and apricots; leaf spot and rust on currants; *Didymella applanata* on raspberries; *Mycosphaerella fragariae* and *Diplocarpon earliana* on strawberries; *Plasmopara viticola* on vines; downy mildew on hops; scab and *Phomopsis citri* on citrus fruit; *Ascochyta chrysanthemi* on chrysanthemums under glass; *Glomerella cingulata* on coffee; *Marssonina* leaf spot on poplars; etc. Applied at 1400 g/ha (hops), 525 g/ha (pome and stone fruit), 560 g/ha (vines). **Phytotoxicity** Slight russetting may occur on some apple varieties, such as Golden Delicious. **Formulation types** SC; WG; WP. **Compatibility** Incompatible with petroleum oils, alkaline materials, and sulfur-containing compounds. **Selected products** 'Delan' (BASF); 'Ditianroc' (Rocca); **mixtures** 'Aktuan' (+ cymoxanil) (BASF, Stähler).

ANALYSIS: **Product** analysis by hplc or by colorimetry (CIPAC Handbook, 1995, G, 50-55; 1985, 1C, 2105; AOAC Methods, 17th Ed., 995.01; E. Amodori & W. Heupt, *Anal. Methods Pestic. Plant Growth Regul.*, 1978, 10, 181). **Residues** determined by hplc or by colorimetry (*idem, ibid.*). Details from BASF.

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 65, 67 (see part 2 of the Bibliography). **Oral** Acute oral LD₅₀ for rats 678, guinea pigs 115 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >2000 mg/kg. Mild skin and eye irritant. **Inhalation** LC₅₀ (4 h) for rats 2.1 mg/l air.

NOEL (2 y) for rats 20, dogs 40 mg/kg diet; for mice 2.8 mg/kg daily. ADI (JMPR) 0.01 mg/kg b.w. [1992]. **Toxicity class** WHO (a.i.) III; EPA (formulation) III **EC classification** Xn; R22| N; R50, R53

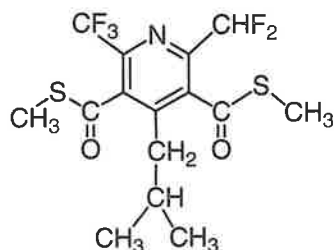
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for male quail 430, female quail 290 mg/kg. **Fish** Toxic to fish; LC₅₀ (96 h) for common carp 0.1 mg/l. **Daphnia** LC₅₀ (24 h) 2.4 mg/l. **Algae** EC₅₀ (96 h) 12 mg/l. **Bees** Contact LD₅₀ >0.1 mg/bee. **Worms** LC₅₀ (7 d) 588.4 mg/kg, (14 d) 578.4 mg/kg. **Other beneficial spp.** Low hazard to predatory mites.

ENVIRONMENTAL FATE: **Soil/Environment** Freundlich K 18–56 mg/kg in soils (o.c. 0.7–2.6%, pH 4.8–6.6).

280 dithiopyr

Herbicide

HRAC K₁ WSSA 3; pyridine



NOMENCLATURE: **Common name** dithiopyr (BSI, ANSI, draft E-ISO)

IUPAC name S,S'-dimethyl 2-difluoromethyl-4-isobutyl-6-trifluoromethylpyridine-3,5-dicarbothioate

Chemical Abstracts name S,S'-dimethyl 2-(difluoromethyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-3,5-pyridinedicarbothioate

CAS RN [97886-45-8] **Development codes** MON 7200 (Monsanto); MON 15 100 (Monsanto); RH 101664 (Rohm & Haas)

PHYSICAL CHEMISTRY: **Mol. wt.** 401.4 **M.f.** C₁₅H₁₆F₅NO₂S₂ **Form** Colourless crystals.

M.p. 65°C **V.p.** 0.53 mPa (25°C) **K_{ow}** logP = 4.75 **Henry** 0.153 Pa m³ mol⁻¹

S.g./density 1.41 (25°C) **Solubility** In water 1.4 mg/l (20°C). **Stability** Stable to hydrolysis.

Aqueous photolysis DT₅₀ 17.6–20.6 d.

COMMERCIALISATION: **History** Herbicide introduced by Monsanto Co. and subsequently sold to Rohm and Haas Co. (now Dow AgroSciences) in 1994. **Patents** US 4692184 **Manufacturers** Dow AgroSciences.

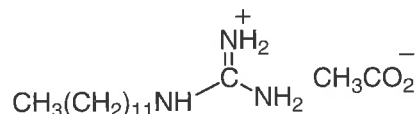
APPLICATIONS: **Biochemistry** Inhibits cell division by disrupting spindle microtubule formation.

Mode of action Pre-emergence herbicide. **Uses** Pre-emergence and early post-emergence control of annual grass and broad-leaved weeds in turf, at 0.25–1.0 lb/a. **Formulation types** EC; GR; Granular on fertiliser. **Selected products** 'Dimension' (Dow AgroSciences).

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats and mice >5000 mg/kg.

Skin and eye Acute percutaneous LD₅₀ for rabbits and rats >5000 mg/kg. Non-irritating to skin;

FRAC M7; multi-site: guanidine

**NOMENCLATURE:** *dodine***Common name** dodine (BSI, E-ISO, (f) F-ISO, ANSI); doguadine (France); tsitrex* (former exception, USSR); dodine acetate* (BSI, before 1969)**IUPAC name** 1-dodecylguanidinium acetate**Chemical Abstracts name** dodecylguanidine monoacetate**CAS RN** [2439-10-3] **EC no.** 219-459-5 **Development codes** CL 7521; AC 5223 (both Cyanamid); BAS 365 F (BASF)**dodine free base****Common name** guanidine (JMAF); dodine* (BSI, before 1969)**CAS RN** [112-65-2]**PHYSICAL CHEMISTRY:** *dodine***Mol. wt.** 287.4 **M.f.** C₁₅H₃₃N₃O₂ **Form** Colourless crystals. **M.p.** 136°C **V.p.** <1 × 10⁻² mPa (20°C) **Solubility** In water 630 mg/l (25°C). Readily soluble in mineral acids, soluble in hot water and in alcohols: in butane-1,4-diol, *n*-butanol, cyclohexanol, *N*-methylpyrrolidone, *n*-propanol, tetrahydrofurfuryl alcohol >250 g/l. Insoluble in most organic solvents. **Stability** Stable in neutral, and moderately alkaline or acidic media, but the free base is liberated by concentrated alkali.**dodine free base****Mol. wt.** 227.4 **M.f.** C₁₃H₂₉N₃**COMMERCIALISATION:** **History** Fungicide reported by B. Cation (*Plant Dis. Rep.*, 1957, 41, 1029). Introduced by American Cyanamid Co. (now BASF AG). **Patents** US 2867562**Manufacturers** Agriphar; Agrokémia; Chemia; General Quimica; Sharda.**APPLICATIONS:** *dodine***Mode of action** Foliar fungicide with protective and some curative action. **Uses** Dodine is used for control of scab on apples, pears, and pecans; leaf spot diseases of cherries, olives, blackcurrants, celery, and other crops; and foliar diseases of strawberries. Also used on other fruit, vegetable, nut, and ornamental crops, and on shade trees. Applied at 30–80 g/100 l (0.25–1.5 kg/ha).**Phytotoxicity** Peaches, plums, vines, and raspberries may be injured. Russetting may occur on some varieties of apple (including Golden Delicious). **Formulation types** SC; SL; WP.**Compatibility** Incompatible with anionic surfactants, chlorobenzilate, lime sulfur, oils, oil emulsions, and hard water. **Selected products** 'Cyprex' (BASF); 'Melprex' (BASF); 'Venturrol' (BASF); 'Dodene' (Sipcam); 'Efuzin' (Agrokémia); 'Guanidol' (Siapa); 'Sulgen' (General Quimica).**ANALYSIS:** **Product** analysis by titration in non-aqueous media (*CIPAC Handbook*, 1983, 1B, 1802; *AOAC Methods*, 17th Ed., 970.07). **Residues** determined by colorimetry of a complex (*ibid.*, 964.19*; *Pestic. Anal. Man.*, 1979, II; G. L. Sutherland, *Anal. Methods Pestic. Plant Growth Regul. Food Addit.*, 1964, 3, 41).

MAMMALIAN TOXICOLOGY: *dodine*

Reviews FAO/WHO 89, 91 (see part 2 of the Bibliography). **Oral** Acute oral LD₅₀ for male and female rats c. 1000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >1500, rats >6000 mg/kg. Irritating to skin. **NOEL** In 2 y feeding trials, rats receiving 800 mg/kg diet suffered a slight retardation of growth with no effect on reproduction or lactation. **ADI** (JMPPR) 0.1 mg/kg b.w. [2000]. **Toxicity class** WHO (a.i.) III; EPA (formulation) I **EC classification** Xn; R22| Xi; R36/38| N; R50, R53

ECOTOXICOLOGY: *dodine*

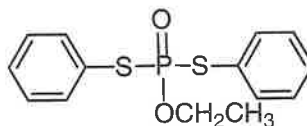
Birds Acute oral LD₅₀ for mallard ducks 1142, Japanese quail 788 mg/kg. **Fish** LC₅₀ for harlequin fish (48 h) 0.53 mg/l; (96 h) 0.6 mg/l. **Daphnia** EC₅₀ (48 h) 0.13 mg/l. **Algae** EC₅₀ for *Selenastrum capricornutum* 5.1 µg/l. **Bees** Topical LD₅₀ for honeybees >0.011 mg/bee.

ENVIRONMENTAL FATE: **Animals** In rats, 95% of the applied dose is eliminated in urine and faeces within 8 days; c. 74% of excreted material is unchanged dodine; metabolites include creatine and guanidine derivatives. **Plants** In plants, dodine is converted to creatine by the action of a methyltransferase and simultaneous oxidative cleavage of the dodecyl moiety.

290 edifenphos

Fungicide

FRAC 6, F2; phosphorothiolate



NOMENCLATURE: **Common name** edifenphos (BSI, E-ISO, (m) F-ISO); EDDP (JMAF)

IUPAC name O-ethyl S,S-diphenyl phosphorodithioate

Chemical Abstracts name O-ethyl S,S-diphenyl phosphorodithioate

CAS RN [17109-49-8] **EC no.** 241-178-1 **Development codes** Bayer 78 418;

SRA 7847 (Bayer)

PHYSICAL CHEMISTRY: **Mol. wt.** 310.4 **M.f.** C₁₄H₁₅O₂PS₂ **Form** Yellow to light brown liquid, with a characteristic odour. **M.p.** -25°C **B.p.** 154°C/1 Pa **V.p.** 3.2 × 10⁻² mPa (20°C) **K_{ow}** logP = 3.83 (20°C) **Henry** 2 × 10⁻⁴ Pa m³ mol⁻¹ (20°C) **S.g./density** 1.251 g/cm³ (20°C) **Solubility** In water 56 mg/l (20°C). In *n*-hexane 20–50, dichloromethane, isopropanol, toluene 200 (all in g/l, 20°C). Readily soluble in methanol, acetone, benzene, xylene, carbon tetrachloride and dioxane. Sparingly soluble in heptane. **Stability** Stable in neutral media. Hydrolysed by strong acids and alkalis; at 25°C, DT₅₀ 19 d (pH 7), 2 d (pH 9). Degradable in the presence of light. **F.p.** 115°C (tech.) (DIN 51755)

COMMERCIALISATION: **History** Fungicide reported by H. Scheinpflug & H. F. Jung (*Pflanzenschutz-Nachr. (Engl. Ed.)*, 1968, **21**, 79). First introduced in 1966. **Patents** BE 686048; DE 1493736 **Manufacturers** Bayer CropScience; Hanwha.

APPLICATIONS: **Biochemistry** Inhibition of phospholipid biosynthesis. **Mode of action** Foliar fungicide with protective and curative action (O. Kodama et al., *Agric. Biol. Chem.*, 1980, **44**, 1015). **Uses** Control of rice blast, at 0.45–0.8 kg/ha. Also controls ear blight and stem rot in rice.

edifenphos 357

primarily through foliar uptake, with little or no soil activity. **Uses** Post-emergence control of wild mustard, hempnettle and other broad-leaved weeds in oilseed rape, at 15–20 g/ha.

Formulation types WG. **Selected products** 'Muster' (DuPont).

ANALYSIS: **Product** and **residue** analysis by hplc/ms/ms (*Handbook of Residue Analytical Methods*, pp. 400–410).

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >2000 mg/kg. Non-irritating to skin; mild irritant of eyes (rabbits). Non-sensitising to skin (guinea pigs). **Inhalation** LC₅₀ (4 h) for rats >5.7 mg/l air. **NOEL** (90 d) for rats and mice >5000 ppm; (2 y) for rats 500 ppm; (1 y) for dogs 3000 ppm; (18 mo) for mice >5000 ppm. Non-oncogenic and non-mutagenic in rats. Non-teratogenic in rats and rabbits. **ADI** 0.235 mg/kg b.w. **Toxicity class** WHO (a.i.) U (company classification)

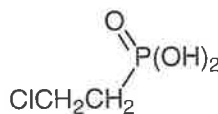
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail 2500, mallard ducks >2250 mg/kg. Dietary LC₅₀ (8 d) for bobwhite quail and mallard ducks >5620 mg/kg diet. **Fish** LC₅₀ (96 h) for bluegill sunfish and rainbow trout >600 mg/l. **Daphnia** LC₅₀ (48 h) >550 mg/l. **Bees** Acute contact toxicity to honeybees >12.5 µg/bee. **Worms** Contact LD₅₀ (14 d) for earthworms >1000 mg/kg soil.

ENVIRONMENTAL FATE: **Animals** Ethametsulfuron-methyl, administered to male and female rats, was rapidly metabolised and excreted in the urine and faeces. Half-lives for excretion range from 12 hours in male rats to 21–26 hours in female rats. Less than 0.2% of the dose remains in the tissues five days after dosing at the highest dose level. No preferential accumulation of ethametsulfuron-methyl or its metabolites. **Plants** Oilseed rape was treated with 30 g/ha ethametsulfuron-methyl in a glasshouse: total radiolabelled residues in the foliage decreased rapidly from c. 1.0 ppm immediately after treatment to 0.02 ppm after 31 days; DT₅₀ 1–3 h. Two primary metabolites were identified, formed by successive dealkylation; firstly of the ethoxy group, to give the corresponding hydroxytriazine, then of the methylamino substituent. Total radioactive residue in mature oilseed rape was very low (0.008 to 0.012 ppm). No ethametsulfuron-methyl was detected in the seed. **Soil/Environment** Soil metabolism (aerobic, lab.) DT₅₀ 9 w; three major metabolites were identified. In soil photolysis studies, sunlight accelerated degradation three-fold relative to dark controls. Aquatic metabolism (aerobic) DT₅₀ 6 mo, (anaerobic) DT₅₀ 2–9 mo, depending on sediment pH. In laboratory soil mobility studies based on soil TLC, soil column leaching, and adsorption/desorption studies, mobility is highly dependent on soil characteristics, primary organic matter content and soil pH. Mobility ranges from very mobile in sandy loam soil to very low mobility in loam soil.

307 ethephon

Plant growth regulator

ethylene generator



NOMENCLATURE: **Common name** ethephon (ANSI, Canada); chorethephon (New Zealand)
IUPAC name 2-chloroethylphosphonic acid

ethephon 377

Chemical Abstracts name (2-chloroethyl)phosphonic acid
CAS RN [16672-87-0] **EC no.** 240-718-3

PHYSICAL CHEMISTRY: **Mol. wt.** 144.5 **M.f.** C₂H₆ClO₃P **Form** Colourless solid; (tech. is a clear liquid). **M.p.** 74–75 °C **B.p.** c. 265 °C (decomp.) **V.p.** <0.01 mPa (20 °C) **K_{ow} logP** <-2.20 (25 °C, unstated pH) **Henry** <1.55 × 10⁻⁹ Pa m³ mol⁻¹ (calc.)
S.g./density 1.409±0.02 (20 °C) (tech.) **Solubility** In water c. 1 kg/l (23 °C). Readily soluble in methanol, ethanol, isopropanol, acetone, diethyl ether, and other polar organic solvents. Sparingly soluble in non-polar organic solvents such as benzene and toluene. Insoluble in kerosene and diesel oil. **Stability** Stable in aqueous solutions having pH <5; at higher pH, decomposition occurs with the liberation of ethylene; DT₅₀ 2.4 d (pH 7, 25 °C). Sensitive to u.v. irradiation. **pKa** pKa₁ 2.5, pKa₂ 7.2

COMMERCIALISATION: **History** Plant growth regulator introduced by Amchem Products Inc. (now Bayer CropScience). **Patents** US 3879188; US 3896163; US 3897486
Manufacturers Agrochem; Bayer CropScience; Cedar; Griffin; Sharda.

APPLICATIONS: **Mode of action** Plant growth regulator with systemic properties. Penetrates into the plant tissues, and is decomposed to ethylene, which affects the growth processes. **Uses** To promote pre-harvest ripening in apples, currants, blackberries, blueberries, cranberries, morello cherries, citrus fruit, figs, tomatoes, sugar beet and fodder beet seed crops, coffee, capsicums, etc.; to accelerate post-harvest ripening in bananas, mangoes, and citrus fruit; to facilitate harvesting by loosening of the fruit in currants, gooseberries, cherries, and apples; to increase flower bud development in young apple trees; to prevent lodging in cereals, maize, and flax; to induce flowering of Bromeliads; to stimulate lateral branching in azaleas, geraniums, and roses; to shorten the stem length in forced daffodils; to induce flowering and regulate ripening in pineapples; to accelerate boll opening in cotton; to modify sex expression in cucumbers and squash; to increase fruit setting and yield in cucumbers; to improve the sturdiness of onion seed crops; to hasten the yellowing of mature tobacco leaves; to stimulate latex flow in rubber trees, and resin flow in pine trees; to stimulate early uniform hull split in walnuts; etc. Maximum application rate per season 2.18 kg/ha for cotton, 0.72 kg/ha for cereals, 1.44 kg/ha for fruit. **Formulation types** EC; SL.

Compatibility Incompatible with alkaline materials and with solutions containing metal ions, e.g. iron-, zinc-, copper-, and manganese-containing fungicides. **Selected products** 'Agritrel' (Cequisa); 'Cerone' (Bayer CropScience); 'Coolmore' (Barclay); 'Eteroc' (Rocca); 'Ethrel' (Bayer CropScience); 'Super Boll' (Griffin); **mixtures** 'Finish' (+ cyclanilide) (Bayer CropScience); 'Terpal' (+ mepiquat chloride) (BASF, DuPont, Bayer CropScience).

ANALYSIS: **Product** analysis by measuring the ethylene, or phosphate ion, produced on treatment with concentrated alkali (CIPAC Handbook, 1998, H, 165). **Residues** determined by conversion to the dimethyl ester, measured by glc with NPD or FPD (Pestic. Anal. Man., Vol. II; Anal. Methods Residues Pestic., 1988, Part II; W. P. Cochrane, J. Assoc. Off. Anal. Chem., 1976, 59, 617).

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 80 (see part 2 of the Bibliography). G. Hennighausen et al., Pharmazie, 1977, 32, 181. **Oral** Acute oral LD₅₀ for rats 3030 mg/kg (tech.). **Skin and eye** Acute percutaneous LD₅₀ for rabbits 1560 mg/kg (tech.). Irritating to skin and eyes. **Inhalation** LC₅₀ (4 h) for rats 4.52 mg/l (tech.). **NOEL** (2 y) for rats 3000 ppm diet. **ADI** (JMPR) 0.05 mg/kg b.w. [1997]. **Toxicity class** WHO (a.i.) U; EPA (formulation) I (tech.)
EC classification Xn; R20/21| C; R34| R52, R53: for preparations containing ≥25%, C; R20/21, R34: for 25%>concn.≥10%, C; R34: for 10%>concn.≥5%, Xi; R36/37/38

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail 1072 mg/kg (tech.). Dietary LC₅₀ (8 d) for bobwhite quail >5000 ppm in diet (tech.). **Fish** LC₅₀ (96 h) for carp >140, rainbow trout 720 mg/l (tech.). **Daphnia** EC₅₀ (48 h) 1000 mg/l (tech.). **Algae** EC₅₀ (24–48 h) for *Chlorella*

378 ethephon

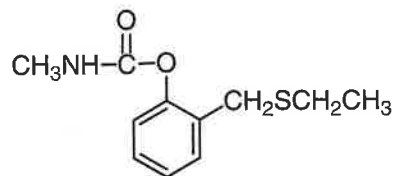
vulgaris 32 mg/l. **Other aquatic spp.** Low toxicity. **Bees** Harmless to bees. **Worms** Not toxic to earthworms.

ENVIRONMENTAL FATE: **Animals** In animals, ethephon is rapidly excreted intact via the urine, and as ethylene via the expired air. **Plants** In plants, ethephon rapidly undergoes degradation to ethylene. **Soil/Environment** Rapidly degraded in soil, and low mobility; unlikely to leach.

308 ethiofencarb

Insecticide

IRAC 1A; carbamate



Main Entries

NOMENCLATURE: **Common name** ethiofencarb (BSI, E-ISO); éthiophencarbe ((*m*) F-ISO)

IUPAC name α -ethylthio-o-tolyl methylcarbamate

Chemical Abstracts name 2-[(ethylthio)methyl]phenyl methylcarbamate

CAS RN [29973-13-5] **EC no.** 249-981-9 **Development codes** HOX 1901;

BAY 108594 (Bayer)

PHYSICAL CHEMISTRY: **Mol. wt.** 225.3 **M.f.** C₁₁H₁₅NO₂S **Form** Colourless crystals; (tech. is a yellow oil, with a mercaptan-like odour). **M.p.** 33.4°C **B.p.** Decomposes on distillation

V.p. 0.45 mPa (20°C); 0.94 mPa (25°C); 26 mPa (50°C) **K_{ow}** logP = 2.04

S.g./density 1.231 (20°C) **Solubility** In water 1.8 g/l (20°C). In dichloromethane, isopropanol and toluene >200, hexane 5-10 (all in g/l, 20°C). **Stability** Stable in neutral and acidic media, but hydrolysed in alkaline solution. In isopropanol/water (1:1), DT₅₀ (37-40°C) 330 d (pH 2), 450 h (pH 7), 5 min (pH 11.4). In aqueous solution, photodegradation in sunlight is very rapid.

F.p. 123°C

COMMERCIALISATION: **History** Insecticide reported by J. Hammann & H. Hoffmann (*Pflanzenschutz-Nachr. (Engl. Ed.)*, 1974, **27**, 267). Introduced by Bayer AG. **Patents** DE 1910588; BE 746649 **Manufacturers** Bayer CropScience.

APPLICATIONS: **Biochemistry** Cholinesterase inhibitor. **Mode of action** Systemic insecticide with contact and stomach action. Absorbed by the leaves and roots. **Uses** Control of aphids on pome fruit, stone fruit, soft fruit, vegetables, ornamentals and sugar beet, at 400-600 g/ha.

Phytotoxicity Phytotoxic to anthurium and begonias. **Formulation types** EC; EW; GR.

Selected products 'Croneton' (Bayer CropScience).

ANALYSIS: **Product** analysis by hplc with u.v. determination (*CIPAC Handbook*, 1992, **E**, 84-88).

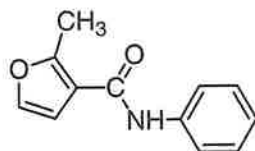
Residues determined by glc (G. Drager, *Pflanzenschutz-Nachr. (Engl. Ed.)*, 1974, **27**, 144); *Anal. Methods Residues Pestic.*, Part I, M13). Methods for the determination of residues are available from Bayer CropScience.

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 38, 39 (see part 2 of the Bibliography).

Oral Acute oral LD₅₀ for male and female rats c. 200, male and female mice c. 240, female dogs >50 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for male and female rats >1000 mg/kg.

ethiofencarb 379

FRAC 7, C2; carboxamide

**NOMENCLATURE:** **Common name** fenfuram (BSI, E-ISO); fenfurame ((m) F-ISO)**IUPAC name** 2-methyl-3-furanilide**Chemical Abstracts name** 2-methyl-N-phenyl-3-furancarboxamide**CAS RN** [24691-80-3] **Development codes** VWL 22 361 (Shell)

PHYSICAL CHEMISTRY: **Mol. wt.** 201.2 **M.f.** C₁₂H₁₁NO₂ **Form** Colourless crystals; (tech., cream solid). **M.p.** 109–110°C (tech.) **V.p.** 0.020 mPa (extrapolated to 20°C) **Henry** 4.02 × 10⁻⁵ Pa m³ mol⁻¹ (calc.) **Solubility** In water 0.1 g/l (20°C). In acetone 300, cyclohexanone 340, methanol 145, xylene 20 (all in g/l, 20°C). **Stability** Stable to heat and light. Stable in neutral media, but hydrolysed by strong acids and alkalis.

COMMERCIALISATION: **History** Fungicide discovered by Shell Research Ltd and developed by KenoGard VT AB (now Bayer CropScience). **Patents** GB 1215066 (to Shell) **Manufacturers** Bayer CropScience.

APPLICATIONS: **Biochemistry** Inhibits mitochondrial function by disrupting complex II (succinate dehydrogenase) in the respiratory electron transport chain. **Uses** Control of bunts and smuts (*Tilletia* and *Ustilago* spp.) in cereals, when applied as a seed treatment. **Formulation types** DS; LS.

ANALYSIS: **Product** analysis by glc with FID. **Residues** in barley and wheat determined by glc.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats 12 900, cats 2450 mg/kg. **Inhalation** LC₅₀ (4 h) for rats >10.3 mg/l air. **NOEL** (2 y) for rats 10 mg/kg daily; (90 d) for dogs 300 mg/kg diet. **Other** Acute i.p. LD₅₀ for rats 1490 mg/kg. Non-mutagenic in the Ames test. **Toxicity class** WHO (a.i.) U; EPA (formulation) IV

ECOTOXICOLOGY: **Fish** LC₅₀ for guppies 11.0 mg/l. **Bees** Not toxic to bees, when used as directed.

ENVIRONMENTAL FATE: **Animals** In rats, following oral administration, up to 83% is eliminated within 16 hours, principally in the urine. **Soil/Environment** DT₅₀ in soil c. 42 d.

ENVIRONMENTAL FATE: EHC 64 (WHO, 1986; a review of carbamate insecticides in general). **Animals** In rats, the major metabolic path is ring hydroxylation to form ethyl [2-[*p*-(*p*-hydroxy=phenoxy)phenoxy]ethyl]carbamate. **Plants** Rapidly degraded in plants. **Soil/Environment** Low mobility in soil, no bioaccumulation. Relatively fast degradation in soil and water; DT₅₀ 1.7–2.5 mo (lab.), few to 31 d (field).

341 fenpiclonil

Fungicide

FRAC 12, E2; phenylpyrrole



Main Entries

NOMENCLATURE: **Common name** fenpiclonil (BSI, draft E-ISO)
IUPAC name 4-(2,3-dichlorophenyl)pyrrole-3-carbonitrile
Chemical Abstracts name 4-(2,3-dichlorophenyl)-1H-pyrrole-3-carbonitrile
CAS RN [74738-17-3] **Development codes** CGA 142 705 (Ciba-Geigy)

PHYSICAL CHEMISTRY: **Mol. wt.** 237.1 **M.f.** C₁₁H₆Cl₂N₂ **Form** White crystals.
M.p. 144.9–151.1°C **V.p.** 1.1 × 10⁻² mPa (25°C) **K_{ow} logP** = 3.86 (25°C) **Henry** 5.4 × 10⁻⁴ Pa m³ mol⁻¹ (calc.) **S.g./density** 1.53 (20°C) **Solubility** In water 4.8 mg/l (25°C). In ethanol 73, acetone 360, toluene 7.2, *n*-hexane 0.026, *n*-octanol 41 (all in g/l, 25°C). **Stability** Not hydrolysed after 6 hours at 100°C between pH 3 and 9. Stable up to 250°C.

COMMERCIALISATION: **History** Fungicide reported by D. Nevill et al. (Proc. 1988 Br. Crop Prot. Conf. - Pests Dis., 1, 65). Introduced in Switzerland (1988) by Ciba-Geigy AG (now Syngenta AG). **Patents** EP 236272

APPLICATIONS: **Biochemistry** Inhibits MAP kinase, in osmotic signal transduction.

Mode of action Slightly systemic, contact fungicide with long-lasting activity. **Uses** Effective against seed-borne pathogens of cereals, especially *Fusarium nivale* and *Tilletia caries*. On non-cereal crops, controls a wide range of seed- and soil-borne fungi (*Alternaria*, *Ascochyta*, *Aspergillus*, *Fusarium*, *Helminthosporium*, *Rhizoctonia* and *Penicillium* spp.). Having a different mode of action, fenpiclonil gives good control of all isolates of *F. nivale*, including those resistant to carbendazim and related fungicides. On cereals and peas, used at 20 g/100 kg seed; on potatoes, at 20–50 g/t (depending on target pathogens). **Formulation types** DS; FS; WS. **Selected products** 'Beret' (Syngenta).

ANALYSIS: Residue determination by hplc. Details available from Syngenta.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats, mice, and rabbits >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >2000 mg/kg. Non-irritating to eyes and skin (rabbits). Non-sensitising (guinea pigs). **Inhalation** LC₅₀ (4 h) for rats >1.5 mg/l air. **NOEL** for rats 1.25, mice 20, dogs 100 mg/kg b.w. daily. **ADI** 0.0125 mg/kg b.w. **Other** Non-teratogenic and non-mutagenic. **Toxicity class** WHO (a.i.) U

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail >2510 mg/kg. LC₅₀ for mallard ducks >5620, bobwhite quail 3976 ppm. **Fish** LC₅₀ (96 h) for rainbow trout 0.8, carp 1.2, bluegill

fenpiclonil 417

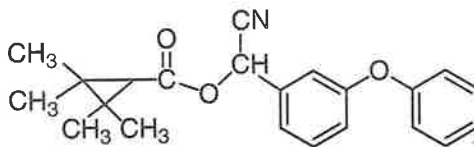
sunfish 0.76, catfish 1.3 mg/l. **Daphnia** LC₅₀ (48 h) 1.3 mg/l. **Algae** LC₅₀ (5 d) for *Scenedesmus subspicatus* 0.22 mg/l. **Bees** Non-toxic to honeybees; LD₅₀ (oral and contact) >5 µg/bee. **Worms** LC₅₀ (14 d) for *Eisenia foetida* 67 mg/kg soil. **Other beneficial spp.** Harmless to carabid beetles.

ENVIRONMENTAL FATE: **Animals** Rapidly absorbed from the gastrointestinal tract into the general circulation; rapidly excreted and almost completely eliminated, mostly in the faeces. The dominant metabolic pathway is oxidation of the pyrrole ring at the 2-position. A minor pathway is hydroxylation of the phenyl ring. All metabolites are excreted as conjugates, mainly as glucuronides. **Plants** Degradation proceeds via oxidation of the pyrrole ring followed by hydrolysis of the nitrile group. Opening of the pyrrole ring and hydroxylation of the phenyl ring are further degradation steps. The parent is, however, the relevant residue; between 13–15 minor metabolites were also observed. **Soil/Environment** Relatively persistent in soil; formation of bound residues represents the major route for dissipation. In leaching and adsorption/desorption experiments, the compound proved to be immobile in soil, RMF 0.3. Photolytic DT₅₀ in water 70 min.

342 fenpropathrin

Acaricide, insecticide

IRAC 3; pyrethroid



NOMENCLATURE: **Common name** fenpropathrin (BSI, E-ISO, ANSI); fenpropathrine ((*m*) F-ISO)

IUPAC name (*RS*)- α -cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate

Chemical Abstracts name cyano(3-phenoxyphenyl)methyl 2,2,3,3-tetramethylcyclopropane=carboxylate

CAS RN [64257–84–7] racemate; [39515–41–8] unstated stereochemistry **EC no.** 254–485–0

Development codes S-3206 (Sumitomo) **Official codes** OMS 1999

PHYSICAL CHEMISTRY: **Mol. wt.** 349.4 **M.f.** C₂₂H₂₃NO₃ **Form** Yellow-brown solid (tech.).

M.p. 45–50°C **V.p.** 0.730 mPa (20°C) **K_{ow} log P** = 6 (20°C) **S.g./density** 1.15 (25°C)

Solubility In water 14.1 µg/l (25°C). In xylene, cyclohexanone 1000, methanol 337 (all in g/kg,

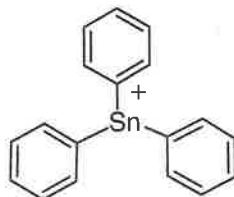
25°C). **Stability** Decomposed in alkaline solutions. Exposure to light and air leads to oxidation and loss of activity.

COMMERCIALISATION: **History** Insecticide reported by Y. Fujita (*Jpn. Pestic. Inf.*, 1981, No. 38, p. 21). Introduced by Sumitomo Chemical Co., Ltd and, in some countries, by Shell International Chemical Co. (now BASF AG). **Patents** GB 1356087; US 3835176 **Manufacturers** Agrochem; Sumitomo.

APPLICATIONS: **Biochemistry** Acts on the nervous system of insects, and disturbs the function of neurons by interaction with the sodium channel. **Mode of action** Acaricide and insecticide with repellent, and contact and stomach action. **Uses** Control of many species of mites (except rust mites) and insects (e.g. whitefly, lepidopterous larvae, leaf miners, leafworms, bollworms, etc.) on pome fruit, citrus fruit, vines, hops, vegetables, ornamentals (including ornamental trees), cotton,

418 fenpropathrin

FRAC 30, C6; organotin fungicide

**NOMENCLATURE:** *fentin*

Common name fentin (BSI, E-ISO); fentine ((f) F-ISO); fenolovo* (former exception, USSR); chemical name is used (Republic of South Africa, USA)

IUPAC name triphenyltin

Chemical Abstracts name triphenylstannylum

CAS RN [668-34-8] **Development codes** VP 1940; Hoe 02824 (Hoechst)

fentin acetate

IUPAC name triphenyltin(IV) acetate; triphenyltin acetate

Chemical Abstracts name (acetyloxy)triphenylstannane

CAS RN [900-95-8] **EC no.** 212-984-0 **Development codes** Hoe 002782 (Hoechst);

AE F002782 (Bayer CropScience) **Official codes** OMS 1020; ENT 25208

fentin hydroxide

IUPAC name triphenyltin(IV) hydroxide; triphenyltin hydroxide

Chemical Abstracts name hydroxytriphenylstannane

CAS RN [76-87-9] **EC no.** 200-990-6 **Development codes** AE F029664 (Bayer CropScience)

Official codes OMS 1017; ENT 28009

PHYSICAL CHEMISTRY: *fentin*

Mol. wt. 350.0 **M.f.** C₁₈H₁₅Sn

fentin acetate

Composition Tech. grade is ≥94% pure. **Mol. wt.** 409.0 **M.f.** C₂₀H₁₈O₂Sn **Form** Colourless crystals. **M.p.** 121–123°C; (tech., 118–125°C) **V.p.** 1.9 mPa (60°C) **K_{ow} logP** = 3.54 **Henry** 2.96 × 10⁻⁴ Pa m³ mol⁻¹ (20°C) (BBA method) **S.g./density** 1.5 (20°C) **Solubility** In water c. 9 mg/l (20°C, pH 5). In ethanol 22, ethyl acetate 82, hexane 5, dichloromethane 460, toluene 89 (all in g/l, 20°C). **Stability** Stable when dry. Converted to fentin hydroxide in the presence of water. Unstable in acids and alkalis (22°C), DT₅₀ <3 h (pH 5, 7 or 9). Decomposed by sunlight and by atmospheric oxygen. **F.p.** 185±5°C (Cleveland open cup)

fentin hydroxide

Composition Tech. grade is ≥95% pure. **Mol. wt.** 367.0 **M.f.** C₁₈H₁₆O₂Sn **Form** Colourless crystals. **M.p.** 123°C **V.p.** 0.0013 mPa (50°C) **K_{ow} logP** = 3.54 **Henry** 6.28 × 10⁻⁷ Pa m³ mol⁻¹ (20°C) **S.g./density** 1.54 at 20°C **Solubility** In water c. 1 mg/l (pH 7, 20°C), (greater at lower pH values). In ethanol 32, isopropanol 48, acetone 46, polyethylene glycol 41 (all in g/l, 20°C). **Stability** Stable in the dark at room temperature. Dehydration occurs on heating above 45°C, yielding bis(triphenyltin) oxide, which is stable up to c. 250°C. Slowly decomposed by sunlight, and more rapidly by u.v. light, to give inorganic tin via di- and mono-phenyltin compounds. **F.p.** 174°C (Cleveland open cup)

fentin 425

COMMERCIALISATION: **History** Fungicidal properties of organotin compounds investigated by G. J. M. van der Kerk & J. G. A. Luijten (*J. Appl. Chem.*, 1954, **4**, 314; 1956, **6**, 56) and reviewed by H. Bock (*Residue Rev.*, 1981, **79**, 1). Fentin acetate was introduced by Hoechst AG (now Bayer CropScience) and fentin hydroxide by N.V. Philips-Duphar (now Crompton Corp.), both in 1959/1960.

fentin acetate

Patents US 3499086 (Hoechst)

APPLICATIONS: *fentin acetate*

Biochemistry Multi-site inhibitor, preventing spore germination, and inhibiting metabolism of the fungal organism, in particular respiration. **Mode of action** Non-systemic fungicide with mainly protective action, but also some curative action. Also acts as an algicide and molluscicide.

Uses Control of early and late blights of potatoes (at 200–300 g/ha), leaf spot diseases of sugar beet (at 200–300 g/ha), anthracnose of beans (at 200 g/ha). **Phytotoxicity** Vines, ornamentals, some fruits, and glasshouse crops may be injured. **Formulation types** WP.

Compatibility Incompatible with oil emulsions and EC formulations. **Selected products** 'Suzu' (Nihon Nohyaku); **mixtures** 'Brestan' (+ maneb) (Bayer CropScience).

fentin hydroxide

Biochemistry Multi-site inhibitor, preventing spore germination, and inhibiting metabolism of the fungal organism, in particular respiration. **Mode of action** Non-systemic fungicide with protective and curative action. **Uses** Control of early and late blights of potatoes (at 200–300 g/ha), leaf spot diseases of sugar beet (at 200–300 g/ha), and fungal diseases of soya beans (at 200 g/ha).

Phytotoxicity Non-phytotoxic when used as directed. Tomatoes and apples may be injured. Surfactants, spreaders or stickers should not be used, as this can lead to phytotoxicity.

Formulation types SC; WP. **Compatibility** Not compatible with strongly acidic compounds. Incompatible with oils and liquid formulations. **Selected products** 'Brestan' (Bayer CropScience); 'Super-Tin' (Chiltern, Griffin); 'Suzu-H' (Nihon Nohyaku).

ANALYSIS: **Product** analysis: fentin acetate and hydroxide may be determined by conversion to fentin chloride, followed by rplc with u.v. detection (*CIPAC Handbook*, 1992, **E**, 89–94), or by hydrolysis of fentin acetate to the hydroxide, which is measured by potentiometric titration (*CIPAC Handbook*, 1980, **1A**, 1263, 1266; *AOAC Methods*, 17th Ed., 979.02), or by glc of a derivative (*ibid.*, 984.04; *CIPAC Handbook*, 1983, **1B**, 1837; *ibid.*, 1988, **D**, 95; Van Rossum *et al.*, *Anal. Methods Pestic. Plant Growth Regul.*, 1980, **11**, 227). **Residues** determined by atomic absorption spectrophotometry of total tin (W. H. Evans *et al.*, *Analyst (London)*, 1979, **104**, 16; T. Ferri *et al.*, *Talanta*, 1989, **36**, 513) or by glc of a derivative (H. H. van den Broek *et al.*, *Analyst (London)*, 1988, **113**, 1237; Van Rossum, *loc. cit.*; P. G. Baker *et al.*, *Analyst (London)*, 1980, **105**, 282).

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 62, 64 (see part 2 of the Bibliography).

fentin

ADI (JMPR) 0.0005 mg/kg b.w. [1991].

fentin acetate

Oral Acute oral LD₅₀ for rats 140–298 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits 127 mg/kg. Irritating to skin and mucous membranes on repeated application. **Inhalation** LC₅₀ (4 h) for male rats 0.044, female rats 0.069 mg/l air. **NOEL** (2 y) for dogs 4 mg/kg diet.

ADI 0.0004 mg/kg b.w. **Toxicity class** WHO (a.i.) II; EPA (formulation) II **EC classification** R40| R63| T+; R26| T; R24/25, R48/23| Xi; R37/38, R41| N; R50, R53

Residues determined by glc (R. A. Guinivan & M. R. Gagnon, *J. Assoc. Off. Anal. Chem. Int.*, 1994, **77**, 728).

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 74, 76 (see part 2 of the Bibliography).

Oral Acute oral LD₅₀ for male rats 1100, female rats 674 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >2000 mg/kg. Mild irritant to skin and eyes, but not a skin sensitiser.

Inhalation LC₅₀ for male rats 27, female rats 3.7 mg/l air. **NOEL** (2 y) for rats 10 mg/kg diet; (1 y) for dogs 5 mg/kg diet; (1.5 y) for mice 25 mg/kg diet. **ADI** (JMPR) 0.001 mg/kg b.w. [1995]. **Other** Not mutagenic. **Toxicity class** WHO (a.i.) III **EC classification** R40| R61| Xn; R22| N; R51, R53

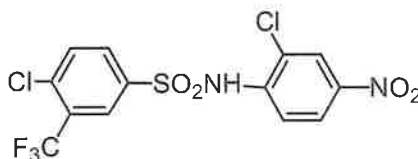
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for mallard ducks >1590 mg/kg. **Fish** LC₅₀ (96 h) for rainbow trout 1.2, bluegill sunfish 1.7 mg/l. **Daphnia** LC₅₀ (48 h) 3.4 mg/l. **Bees** Not toxic to bees. LD₅₀ >150 µg/bee.

ENVIRONMENTAL FATE: **Soil/Environment** Results of several different studies under varying environmental conditions indicate average DT₅₀ 95 d.

394 flusulfamide

Fungicide

FRAC 36, U6; benzenesulfonamide



NOMENCLATURE: **Common name** flusulfamide (BSI, draft E-ISO)

IUPAC name 2',4-dichloro- α,α,α -trifluoro-4'-nitro-*m*-toluenesulfonanilide

Chemical Abstracts name 4-chloro-*N*-(2-chloro-4-nitrophenyl)-3-(trifluoromethyl)benzenesulfonamide

CAS RN [106917-52-6] **Development codes** MTF-651 (Mitsui)

PHYSICAL CHEMISTRY: **Mol. wt.** 415.2 **M.f.** C₁₃H₇Cl₂F₃N₂O₄S **Form** Light yellow crystals.

M.p. 169.7–171.0°C **V.p.** 9.9×10^{-7} mPa (40°C) **K_{ow}** logP = 2.8±0.5

S.g./density 1.739 g/cm³ (23°C) **Solubility** In water 2.9 mg/kg (25°C). In methanol 24, acetone 314, xylene 14, tetrahydrofuran 592 (all in g/kg, 25°C). **Stability** Stable between 35°C and 80°C in the dark for 90 d. Stable in acidic and in alkaline media.

COMMERCIALISATION: **History** Fungicide discovered in 1986 by Mitsui Toatsu Chemicals, Inc. (now Mitsui Chemicals Inc.). **Patents** EP 199433 **Manufacturers** Mitsui.

APPLICATIONS: **Mode of action** Inhibits spore germination. **Uses** Used as a soil treatment for control of *Plasmodiophora brassicae* in brassicas and *Polymyxa betae* (fungal vector of beet yellow vein virus causing rhizomania disease) in sugar beet, at 0.6–0.9 kg/ha. Also controls *Pythium*, *Rhizoctonia*, *Phytophthora*, and *Fusarium* spp. **Formulation types** DP; SC. **Selected products** 'Nebijin' (Mitsui).

ANALYSIS: **Product** analysis by hplc.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for male rats 180, female rats 132 mg/kg.

Skin and eye Acute percutaneous LD₅₀ for male and female rats >2000 mg/kg. Slight eye irritant; not a skin irritant (rabbits). Not a skin sensitiser. **Inhalation** LC₅₀ (4 h) for male and female rats 0.47 mg/l.

484 flusulfamide

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail 66 mg/kg. **Fish** TLm (96 h) for bluegill sunfish 1.2 mg/l. **Daphnia** EC₅₀ (48 h) 0.29 mg/l. **Algae** E_r-C₅₀ (72 h) 4.2 mg/l. **Bees** LD₅₀ >200 µg/bee. **Worms** >9 kg/ha.

ENVIRONMENTAL FATE: **Animals** In rats, the parent compound, 4-chloro-*N*-(2-chloro-4-hydroxyphenyl)-α,α,α-trifluoro-*m*-toluenesulfonamide and 4-chloro-α,α,α-trifluoro-*m*-toluenesulfonamide are found. **Plants** In cabbage, the parent compound, 4-chloro-*N*-(2-chloro-4-formylaminophenyl)-α,α,α-trifluoro-*m*-toluenesulfonamide, 4-chloro-α,α,α-trifluoro-*m*-toluenesulfonamide and 4-chloro-α,α,α-trifluoro-*m*-toluenesulfonate are found.

395 fluthiacet-methyl

Herbicide

HRAC E WSSA 14; thiadiazole



Main Entries

NOMENCLATURE: **Common name** fluthiacet-methyl (BSI, pa ISO)

IUPAC name methyl [2-chloro-4-fluoro-5-(5,6,7,8-tetrahydro-3-oxo-1*H*,3*H*-[1,3,4]thiadiazolo[3,4-*a*]pyridazin-1-ylideneamino)phenylthio]acetate

Chemical Abstracts name methyl [[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]acetate

CAS RN [117337-19-6]; [149253-65-6] acid **Development codes** KIH-9201 (Kumiai); CGA-248,757 (Ciba-Geigy)

PHYSICAL CHEMISTRY: **Mol. wt.** 403.9 **M.f.** C₁₅H₁₅ClFN₃O₃S₂ **Form** White powder.

M.p. 105.0–106.5°C (OECD 102) **V.p.** 4.41 × 10⁻⁴ mPa (25°C) **K_{ow} logP** = 3.77 (25°C)

Henry 2.1 × 10⁻⁴ Pa m³ mol⁻¹ (calc.) **S.g./density** 0.43 (bulk, 20°C) **Solubility** In water 0.85 (distilled), 0.78 (pH 5 & 7), 0.22 (pH 9) mg/l (25°C). In methanol 4.41, acetone 101, toluene 84, *n*-octanol 1.86, acetonitrile 68.7, ethyl acetate 73.5, dichloromethane 9 (all in g/l, 25°C); in *n*-hexane 0.232 g/l (20°C).

Stability In water, DT₅₀ 484.8 d (pH 5), 17.7 d (pH 7), 0.2 d (pH 9). In light, DT₅₀ 4.92 d.

COMMERCIALISATION: **History** Reported by Kumiai Chemical Industry Co., Ltd and Ciba-Geigy AG (now Syngenta AG) (T. Miyazawa et al., *Proc. Br. Crop Prot. Conf. - Weeds*, 1993, **1**, 23). Syngenta divested their interests to Kumiai in 2001. **Patents** US 4885023; US 4906279; EP-B-0273417

Manufacturers Ihara/Kumiai.

APPLICATIONS: **Biochemistry** Protoporphyrinogen oxidase inhibitor, causing accumulation of protoporphyrins, enhancing peroxidation of membrane lipids, and leading to irreversible damage to membrane structure and cellular function. Converted to the active substance in sensitive plants.

Mode of action Selective, contact herbicide, requiring light for activity. **Uses** Post-emergence herbicide for control of broad-leaved weeds (e.g. *Abutilon theophrasti*, *Chenopodium album*, *Amaranthus retroflexus*)

fluthiacet-methyl 485

performance in rats over 3 generations at 1000 mg/kg diet; no teratogenic effect was noted in hamsters, monkeys or rats. **ADI** (JMPR) 0.1 mg/kg b.w. [1995]. **Toxicity class** WHO (a.i.) U; EPA (formulation) IV **EC classification** R40| Xn; R20| Xi; R36| R43| N; R50

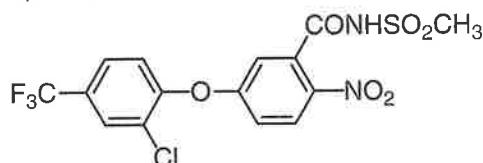
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for mallard ducks >2000 mg/kg. **Fish** Toxic to fish. **Daphnia** EC₅₀ >1.46 mg/l. **Algae** E_bC₅₀ and E_rC₅₀ >10 mg/l. **Other aquatic spp.** Non-toxic to aquatic organisms under practical conditions because of its instability in water. **Bees** Non-toxic to bees; LD₅₀ (oral) >236 µg/bee; (contact) >200 µg/bee. **Worms** Non-toxic. **Other beneficial spp.** Slightly harmful to *Coccinella septempunctata*, harmless to *Poecilus cupreus*, *Trichogramma cacoeciae*, *Chrysoperla carnea*, *Typhlodromus pyri*, *Aleochara bilineata* and *Aphidius rhopalosiphi* (IOBC).

ENVIRONMENTAL FATE: **Animals** Major metabolites are phthalimide, phthalic acid and phthalamic acid. **Plants** As for animals. **Soil/Environment** DT₅₀ (soil) 4.3 d; DT₅₀ (water) <0.7 h. Strongly adsorbed to soil: adsorption K_{oc} 304–1164 (calc.); unlikely to leach.

401 fomesafen

Herbicide

HRAC E WSSA 14; diphenyl ether



NOMENCLATURE: *fomesafen*

Common name fomesafen (BSI, draft E-ISO, ANSI); fomésafène ((m) draft F-ISO)

IUPAC name 5-(2-chloro- α,α,α -trifluoro-*p*-tolxyloxy)-*N*-methylsulfonyl-2-nitrobenzamide

Chemical Abstracts name 5-[2-chloro-4-(trifluoromethyl)phenoxy]-*N*-(methylsulfonyl)-2-nitrobenzamide

CAS RN [72178-02-0] **EC no.** 276-439-9 **Development codes** PP021 (ICI)

fomesafen-sodium

CAS RN [108731-70-0]

PHYSICAL CHEMISTRY: *fomesafen*

Mol. wt. 438.8 **M.f.** C₁₅H₁₀ClF₃N₂O₆S **Form** White crystals. **M.p.** 219°C **V.p.** <4 × 10⁻³ mPa (20°C) **K_{ow}** logP = 2.9 (pH 1), <2.2 (pH 4–10) **Henry** <2 × 10⁻⁷ Pa m³ mol⁻¹ (pH 7, 20°C) **S.g./density** 1.61 (20°C) **Solubility** In pure water c. 50, <10 (pH 1–2), 10 000 (pH 9) (all in mg/l, 20°C). **Stability** Stable in storage for at least 6 months at 50°C. Decomposed by light. Stable at pH 3 and 11 (40°C). Stable to aqueous photolysis for 32 d (pH 7, 25°C). **pKa** 2.83 (20°C); forms water-soluble salts (e.g. fomesafen-sodium)

fomesafen-sodium

Mol. wt. 460.7 **M.f.** C₁₅H₉ClF₃N₂NaO₆S

COMMERCIALISATION: **History** Herbicide reported by S. R. Colby *et al.* (*Proc. Int. Congr. Plant Prot.*, 10th, 1983, 1, 295). Introduced by ICI Plant Protection Division (now Syngenta AG).

Patents EP 3416 **Manufacturers** Sannong; Syngenta.

APPLICATIONS: **Biochemistry** Protoporphyrinogen oxidase inhibitor. **Mode of action** Selective herbicide, absorbed by both leaves and roots, with very limited translocation in the phloem.

Uses Early post-emergence control of broad-leaved weeds in soya beans. Applied at 200–400 g/ha. **Phytotoxicity** Non-phytotoxic to soya beans and to other crops, such as beans of the genus *Phaseolus* and the leguminous cover crops *Pueraria* and *Calapogonium*.

Formulation types ME; SL.

fomesafen-sodium

Selected products 'Flex' (Syngenta); 'Flexstar' (Syngenta); 'Reflex' (Syngenta).

ANALYSIS: **Product** analysis by hplc with u.v. detection. **Residue** analysis in soil by hplc; in crops by tlc, hplc or nmr. Details available from Syngenta.

MAMMALIAN TOXICOLOGY: *fomesafen*

Oral Acute oral LD₅₀ for male rats 1250–2000, female rats 1600 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >1000 mg/kg. Mild skin irritant; mild to moderate eye irritant (rabbits). Extreme skin sensitiser (Magnusson & Kligman test), not a skin sensitiser (ear/flank Stevens test, guinea pigs). **Inhalation** LC₅₀ (4 h) for male rats 4.97 mg/l. **NOEL** (2 y) for rats 5 mg/kg b.w. daily; (18 mo) for mice 1 mg/kg b.w. daily (liver tumours in mice due to peroxisome proliferation - not relevant to man); (6 mo) for dogs 1 mg/kg b.w. daily. **NOEL** developmental toxicity for rabbits 2.5 mg/kg b.w. daily. **ADI** 0.05 mg/kg. **Other** Genotoxicity negative. Not oncogenic. **Toxicity class** WHO (a.i.) III; EPA (formulation) III **EC classification** Xn; R22

fomesafen-sodium

Oral Acute oral LD₅₀ for male rats 1860, female rats 1500 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >780 mg/kg. **Other** Not oncogenic.

ECOTOXICOLOGY: *fomesafen*

Birds Acute oral LD₅₀ for mallard ducks >5000 mg/kg. Dietary LC₅₀ (5 d) for mallard ducks and bobwhite quail >20 000 mg/kg. **Fish** LC₅₀ (96 h) for rainbow trout 170, bluegill sunfish 1507 mg/l. **Daphnia** EC₅₀ (48 h) 0.33 g/l. **Algae** EC₅₀ 170 µg/l. **Bees** Low oral and contact toxicity to bees. LD₅₀ (oral) ≥50 µg/bee; (contact) ≥100 µg/bee. **Worms** LC₅₀ (14 d) >1000 mg/kg.

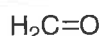
ENVIRONMENTAL FATE: **Plants** In soya beans, the diphenyl ether bond is rapidly cleaved to give inactive metabolites. **Soil/Environment** In soil, degrades slowly under aerobic conditions, DT₅₀ >6 mo, but degrades more rapidly under anaerobic conditions, DT₅₀ <1–2 mo. K_{oc} 34–164. Photodegradation occurs on the soil surface, DT₅₀ 100–104 d. In the field, mean DT₅₀ c. 15 w. No accumulation in lower soil levels; the majority of fomesafen residues are present in the top six inches of soil.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for male rats 2787, female rats 1568, male mice 2218, female mice 2783 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >2000 mg/kg. **Inhalation** LC₅₀ (4 h) for rats: no mortality in saturated atmosphere. **NOEL** 7.5 mg/kg b.w. daily.

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail >2250 ng/kg. Dietary LC₅₀ (5 d) for bobwhite quail >5600 ppm. **Fish** LC₅₀ (96 h) for rainbow trout 9.2 mg/l; (48 h) for carp 8.6 mg/l, for goldfish 10–40 ppm. **Daphnia** LC₅₀ (48 h) 8.0 mg/l. **Algae** EC₅₀ (3 h) 11 mg/l.

404 formaldehyde

Fungicide, bactericide



NOMENCLATURE: **Common name** formaldehyde (BSI, E-ISO, JMAF, accepted in lieu of common name); aldéhyde formique (F-ISO, accepted in lieu of common name)

IUPAC name formaldehyde

Chemical Abstracts name formaldehyde

Other names formalin (37–41% solution) **CAS RN** [50–00–0] **EC no.** 200–001–8

PHYSICAL CHEMISTRY: **Mol. wt.** 30.0 **M.f.** CH₂O **Form** Colourless, flammable gas, with a pungent odour. Formalin is a colourless liquid, with a pungent odour. **M.p.** –92°C **B.p.** –19.5°C **S.g./density** 0.815 (–20°C); 1.081–1.085 (25°C) (formalin) **Solubility** In water 55%. Miscible with acetone, alcohols, and ethers. Formalin miscible with water, acetone, ethanol. **Stability** Highly chemically-reactive. Polymerised in aqueous solution to trioxymethylene (retarded by the addition of methanol). Sensitive to light. Powerful reducing agent. **F.p.** Flammable

COMMERCIALISATION: **History** Introduced as a disinfectant by Loew in 1888 and was first used as a seed disinfectant by Geuther in 1896.

APPLICATIONS: **Mode of action** Fumigant fungicide and bactericide. **Uses** Soil sterilant with bactericidal and fungicidal properties, used in glasshouses (after cropping) and mushroom houses. Also used as a silage preservative. **Phytotoxicity** Extremely phytotoxic. **Formulation types** HN; SL.

ANALYSIS: **Product** analysis by oxidation with hydrogen peroxide to form formic acid which is determined by titration (MAFF Ref. Book, 1958, No. 1, p. 36; CIPAC Handbook, 1985, 1C, 2130; AOAC Methods, 17th Ed., 898.01) or by titration with thiocyanate (*ibid.*, 897.01, 931.03).

Atmospheres may be measured by reaction with chromotropic acid and colorimetry (P. R. Ludlam & J. G. King, *Analyst (London)*, 1981, 106, 488). Methods reviewed by J. L. Daft in *Comp. Analyt. Profiles*, Chapter 11. See also general review by E. R. Kennedy et al. (*Formaldehyde: Analytical Chemistry and Toxicology*, ACS Series, 1985, No. 210, pp. 3–12).

MAMMALIAN TOXICOLOGY: **Reviews** J. W. Goode, *Formaldehyde: Analytical Chemistry and Toxicology*, ACS Series, 1985, No. 210, pp. 217–277. **IARC ref.** 62; **class** 2A **Oral** Acute oral LD₅₀ for rats 550–800 mg/kg (formalin). **Skin and eye** Acute percutaneous LD₅₀ for rabbits 270 mg/kg (formalin). Absorbed through the skin. **Inhalation** LC₅₀ for rats (0.5 h) 0.82 mg/l, (4 h) 0.48 mg/l; for mice (4 h) 0.414 mg/l. Formaldehyde vapour is very irritating to the mucous membranes and is toxic to animals, including man. **Toxicity class** WHO (a.i.) FM **EC classification** R40| T; R23/24/25| C; R34| R43: (for preparations with concn.>25%, T;

R23/24/25, R34, R40, R43: for 25%>concn.≥5%, Xn; R20/21/22, R36/37/38, R40, R43: for 5%>concn.≥1%, Xn; R40, R43: for 1%>concn.≥0.2%, Xi; R43)

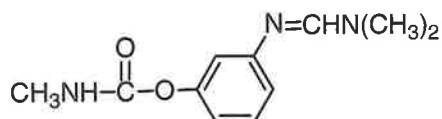
ECOTOXICOLOGY: Fish Toxic to fish.

ENVIRONMENTAL FATE: EHC 89 (WHO, 1989). **Soil/Environment** In the presence of air, formaldehyde is oxidised to formic acid.

405 formetanate

Acaricide, insecticide

IRAC 1A; carbamate



NOMENCLATURE: *formetanate*

Common name formetanate (BSI, E-ISO, (m) F-ISO, ANSI, ESA)

IUPAC name 3-dimethylaminomethyleneaminophenyl methylcarbamate

Chemical Abstracts name *N,N*-dimethyl-*N'*-[3-[[[(methylamino)carbonyl]oxy]phenyl]=methanimidamide

CAS RN [22259-30-9] **EC no.** 244-879-0 **Development codes** SN 36056 (Schering); ZK 10970; EP-332 (AgrEvo)

formetanate hydrochloride

IUPAC name 3-dimethylaminomethyleneaminophenyl methylcarbamate hydrochloride

CAS RN [23422-53-9] **EC no.** 245-656-0 **Development codes** SN 36056HCl (Schering); Hoe 132807 (Hoechst) **Official codes** ENT 27566

PHYSICAL CHEMISTRY: *formetanate*

Mol. wt. 221.3 **M.f.** C₁₁H₁₅N₃O₂ **pKa** 8.0 (25 °C), weak base

formetanate hydrochloride

Mol. wt. 257.8 **M.f.** C₁₁H₁₆ClN₃O₂ **Form** Colourless crystalline powder. **M.p.** 200–202 °C (decomp.) **V.p.** 0.0016 mPa (25 °C) **K_{ow}** logP ≤–2.7 (pH 7–9) **Henry** 5.0 × 10^{–10} Pa m³ mol^{–1} (22 °C) **S.g./density** Bulk density c. 0.5 g/ml. **Solubility** In water 822 g/l (25 °C). In methanol 283, acetone 0.074, toluene 0.01, dichloromethane 0.303, ethyl acetate 0.001, *n*-hexane <0.0005 (all in g/l, 20 °C). **Stability** Stable for at least 8 years at room temperature. Decomposes at c. 200 °C. Hydrolysis DT₅₀ (22 °C) 62.5 d (pH 5), 23 h (pH 7), 2 h (pH 9). Subject to photolytic degradation in aqueous solution, with DT₅₀ 1333 h (pH 5), 17 h (pH 7), 2.9 h (pH 9), corrected for dark controls. **F.p.** Not flammable

COMMERCIALISATION: **History** Acaricidal properties of hydrochloride described by W. R. Steinhausen (Z. Angew. Zool., 1968, 55, 107). Introduced by Schering AG (now Bayer CropScience) and transferred to Margarita Internacional in 2000. **Patents** DE 1169194; GB 987381 **Manufacturers** Margarita.

APPLICATIONS: **Biochemistry** Cholinesterase inhibitor. **Mode of action** Acaricide and insecticide with contact and stomach action.

formetanate 497

Chemical Abstracts name O-ethyl S-(1-methylpropyl) (2-oxo-3-thiazolidinyl)phosphonothioate
CAS RN [98886-44-3] **Development codes** IKI-1145 (Ishihara Sangyo)

PHYSICAL CHEMISTRY: **Mol. wt.** 283.3 **M.f.** C₉H₁₈NO₃PS₂ **Form** Pale yellow liquid; (tech. is a light brown liquid). **B.p.** 198°C/0.5 mmHg **V.p.** 5.6×10^{-1} mPa (25°C) **K_{ow} logP** = 1.68 **Henry** 1.76×10^{-5} Pa m³ mol⁻¹ **S.g./density** 1.240 (20°C) **Solubility** In water 9.85 g/l (20°C). In n-hexane 15.14 g/l (20°C). **Stability** In water, DT₅₀ 3 d (pH 9, 25°C). **F.p.** 127.0°C (Pensky-Martens closed tester)

COMMERCIALISATION: **History** Nematicide discovered by Ishihara Sangyo Kaisha, Ltd and launched in Japan in 1992. **Manufacturers** Ishihara Sangyo.

APPLICATIONS: **Biochemistry** Cholinesterase inhibitor. **Mode of action** Systemic, non-fumigant, soil-applied. **Uses** Control of nematodes (*Meloidogyne* spp., *Heterodera* spp. and *Pratylenchus* spp.), aphids, mites, thrips, etc., in vegetables, potatoes and bananas, etc. Applied at 2.0–5.0 kg/ha. **Formulation types** EC; FG. **Selected products** 'Cierito' (Ishihara Sangyo); 'Nemathorin' (Ishihara Sangyo, Syngenta).

ANALYSIS: Details from Ishihara Sangyo.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for male rats 73, female rats 57 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for male rats 2396, female rats 861 mg/kg. Irritating to eyes; not irritating to skin (rabbits). Sensitising to skin (guinea pigs). **Inhalation** LC₅₀ (4 h) for male rats 0.832, female rats 0.558 mg/l. **EC classification** T; R23/25, R39| Xn; R21| Xi; R41| R43| N; R50, R53

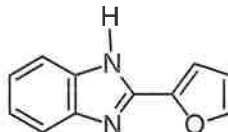
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for ducks 20, quail 10 mg/kg. **Fish** LC₅₀ (96 h) for trout 114, bluegill sunfish 171 mg/l. **Daphnia** EC₅₀ (48 h) 279 µg/l. **Bees** LD₅₀ (48 h) 0.256 µg/bee.

ENVIRONMENTAL FATE: EHC 63 (WHO, 1986; a general review of organophosphorus insecticides).

409 fuberidazole

Fungicide

FRAC 1, B1; benzimidazole



NOMENCLATURE: **Common name** fuberidazole (BSI, E-ISO, (m) F-ISO); no name (Canada)

IUPAC name 2-(2-furyl)benzimidazole

Chemical Abstracts name 2-(2-furanyl)-1H-benzimidazole

Other names furidazol; furidazole **CAS RN** [3878-19-1] **EC no.** 223-404-0

Development codes Bayer 33 172; W VII/117

PHYSICAL CHEMISTRY: **Mol. wt.** 184.2 **M.f.** C₁₁H₈N₂O **Form** Fine crystalline, light brown, odourless powder (tech.). **M.p.** 292°C (decomp.) **V.p.** 9×10^{-4} mPa (20°C); 2×10^{-3} mPa

502 fuberidazole

(25°C) $K_{ow} \log P = 2.67$ (22°C) **Henry** $2 \times 10^{-6} \text{ Pa m}^3 \text{ mol}^{-1}$ (20°C) **Solubility** In water 220 mg/l (pH 4), 71 mg/l (pH 7) (both 20°C). In isopropanol 31, toluene 0.35, dichloromethane 6.6 (all in g/l, 20°C). **Stability** Stable to hydrolysis in pure water, under sterile conditions, but sensitive to light; DT₅₀ 15 min (aqueous solution), 6 h (on silica gel). **pKa** c. 4, weak base

COMMERCIALISATION: **History** Its preparation described by R. Weidenhagen (*Ber. Dtsch. Chem. Ges.*, 1936, **69**, 2271) and its fungicidal activity by G. Schuhmann (*Nachrichtenbl. Dtsch. Pflanzenschutzdienstes (Braunschweig)*, 1968, **20**, 1). Introduced by Bayer AG. **Patents** DE 1209799 **Manufacturers** Bayer CropScience.

APPLICATIONS: **Biochemistry** Inhibits mitosis by binding to beta-tubuline.

Mode of action Systemic fungicide with specific action against *Fusarium*. **Uses** Seed treatment for control of *Fusarium* spp. in cereals, at 4.5 g/100 kg seed; only in combination with other fungicides.

Formulation types DS; FS; LS; WS. **Selected products mixtures** 'Baytan C' (+ imidacloprid + triadimenol) (seed treatment) (Bayer CropScience); 'Baytan Combi' (+ imazalil + triadimenol) (fuberidazole not present in some formulations) (Bayer CropScience); 'Baytan Secur' (+ imidacloprid + triadimenol) (seed treatment) (Bayer CropScience); 'Baytan Spezial' (+ triadimenol) (seed treatment) (Bayer CropScience); 'Baytan Universal' (+ imazalil + triadimenol) (seed treatment) (Bayer CropScience).

ANALYSIS: **Product** analysis by u.v. spectroscopy; details available from Bayer CropScience.

Residues determined by glc (W. Specht, *Pflanzenschutz-Nachr. (Engl. Ed.)*, 1977, **30**, 55; W. Specht & M. Tillkes, *ibid.*, 1980, **33**, 61). Methods for the determination of residues are also available from Bayer CropScience.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for male rats c. 336, mice c. 650 mg/kg.

Skin and eye Acute percutaneous LD₅₀ for rats >2000 mg/kg. Not irritating to skin and eyes (rabbits). **Inhalation** LC₅₀ (4 h) for rats >0.3 mg/l air (aerosol). **NOEL** (2 y) for male rats 80, female rats 400, dogs 20, mice 100 mg/kg diet. **ADI** (company proposed) 0.005 mg/kg b.w. **Toxicity class** WHO (a.i.) II **EC classification** Xn; R22| N; R50, R53

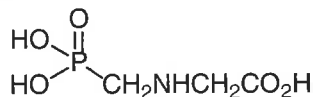
ECOTOXICOLOGY: **Birds** LD₅₀ for Japanese quail 750 mg/kg b.w. Dietary LC₅₀ (5 d) for Japanese quail >5000 mg/kg diet. **Fish** LC₅₀ (96 h) for rainbow trout 0.91, bluegill sunfish 4.3 mg/l. **Daphnia** EC₅₀ 4.7 mg/l. **Algae** E_rC₅₀ for *Pseudokirchneriella subcapitata* 12.1 mg/l. **Bees** LD₅₀ (oral) >187.2 µg/bee; (contact) >200 µg/bee. **Worms** LC₅₀ for *Eisenia foetida* >1000 mg/kg dry soil. **Other beneficial spp.** No effect on *Aphidius rhopalosiphii* or *Typhlodromus pyri* up to 26 g/ha.

ENVIRONMENTAL FATE: **Animals** In rats, fuberidazole is widely distributed and completely excreted within 72 hours via both urine and faeces. Metabolism is almost complete (>97%) via hydroxylation, followed by conjugation and/or cleavage of the furan ring, and oxidation.

Plants According to a balance study with labelled a.i. using seed-treated spring wheat planted in a lysimeter, young plants absorbed about 10% of the applied radioactivity which, however, decreased to 1–2% in later development stages. **Soil/Environment** Mobility in different soils is low. Degradation is rapid; DT₅₀ 5.8–14.7 d, DT₉₀ 19.3–49 d, measured in laboratory trials using predominantly BBA standard soils 1 and 2. Direct photodegradation in water contributes to overall elimination of fuberidazole from the environment to a great extent; DT₅₀ <1 d. Volatilisation into the air of the parent compound, or degradation products, could not be observed in the balance study described under Plants.

fuheridazole 503

HRAC G WSSA 9; glycine derivative



For a general review, see "Glyphosate, A Unique Global Herbicide".

NOMENCLATURE: *glyphosate***Common name** glyphosate (BSI, E-ISO, (m) F-ISO, ANSI, WSSA, JMAF)**IUPAC name** N-(phosphonomethyl)glycine**Chemical Abstracts name** N-(phosphonomethyl)glycine**CAS RN** [1071-83-6] **EC no.** 213-997-4 **Development codes** MON-0573 (Monsanto); CP 67573 (Monsanto)*glyphosate-ammonium***CAS RN** [40465-66-5] monoammonium salt; [69254-40-6] diammonium salt; [114370-14-8] unspecified ammonium salt **Development codes** MON 8750 (Monsanto)*glyphosate-isopropylammonium***CAS RN** [38641-94-0] **EC no.** 254-056-8 **Development codes** MON 0139 (Monsanto); MON 77209 (Monsanto)*glyphosate-sodium***CAS RN** [34494-03-6] **Development codes** MON 8722 (Monsanto)*glyphosate-trimesium***IUPAC name** trimethylsulfonium N-(phosphonomethyl)glycinate**Chemical Abstracts name** N-(phosphonomethyl)glycine trimethylsulfonium salt**Other names** sulfosate **CAS RN** [81591-81-3] **Development codes** SC 0224; ICIA0224 (ICI)**PHYSICAL CHEMISTRY:** *glyphosate***Composition** Tech. is $\geq 95\%$ pure. Zwitterion structure (P. Knuuttila & H. Knuuttila, *Acta Chem. Scand.*, 1979, **33**, 623). **Mol. wt.** 169.1 **M.f.** $\text{C}_3\text{H}_8\text{NO}_5\text{P}$ **Form** Colourless crystals.**M.p.** $189.5 \pm 0.5^\circ\text{C}$ **B.p.** Decomp. $> 200^\circ\text{C}$ **V.p.** 1.31×10^{-2} mPa (25°C) **K_{ow} logP** < -3.2 (pH 2-5, 20°C), (OECD 107; EEC A8) **Henry** $< 2.1 \times 10^{-7}$ Pa $\text{m}^3 \text{mol}^{-1}$ **S.g./density** 1.705 (20°C) **Solubility** In water 10.5 g/l (pH 1.9, 20°C). Insoluble in common organic solvents, e.g. acetone, ethanol and xylene. The alkali-metal and amine salts are readily soluble in water. **Stability** Glyphosate and all its salts are non-volatile, do not photochemically degrade and are stable in air. Glyphosate is stable to hydrolysis at pH 3, 6 and 9 ($5-35^\circ\text{C}$). **pKa** 2.34 (20°C), 5.73 (20°C), 10.2 (25°C) **F.p.** Not flammable*glyphosate-ammonium***Composition** Tech. is 95.2% pure. **Mol. wt.** 186.1 **M.f.** $\text{C}_3\text{H}_{11}\text{N}_2\text{O}_5\text{P}$ **Form** Odourless, white powder. **M.p.** Decomp. $> 190^\circ\text{C}$, without melting **V.p.** 9×10^{-3} mPa (25°C) **K_{ow} logP** < -3.7 **Henry** 1.16×10^{-8} Pa $\text{m}^3 \text{mol}^{-1}$ (calc.) **S.g./density** 1.433 (22°C) **Solubility** In water 144 ± 19 g/l (pH 3.2). Essentially insoluble in organic solvents. **Stability** Stable over 5 days at 50°C (pH 4, 7 and 9). **pKa** See isopropylammonium salt **F.p.** Not flammable

glyphosate-isopropylammonium

Composition As a wet cake, contains c. 62% w/w isopropylamine salt, c. 35% water.

Mol. wt. 228.2 **M.f.** $C_6H_{17}N_2O_5P$ **Form** Odourless, white powder. **M.p.** Occurs in 2 steps,

143–164 °C and 189–223 °C **B.p.** Decomposes without boiling **V.p.** 2.1×10^{-3} mPa (25 °C)

K_{ow} $\log P = -5.4$ **Henry** 4.6×10^{-10} Pa m³ mol⁻¹ (25 °C, calc.) **S.g./density** 1.482 (20 °C)

Solubility In water 1050 g/l (25 °C, pH 4.3). In dichloromethane <0.5, methanol 19.86 (both in g/l, 20 °C). **Stability** Stable 5 days at pH 4, 5, and 9 (50 °C). **pKa** 5.77 ± 0.03 , 2.18 ± 0.02 (20 ± 2 °C),

(OECD 112)

glyphosate-sodium

Mol. wt. 191.1 **M.f.** $C_3H_7NNaO_5P$ **Form** Odourless, white powder. **M.p.** Decomp. >260 °C

V.p. 7.56×10^{-3} mPa (25 °C) **K_{ow}** $\log P < -3.02$ **Henry** 4.27×10^{-9} Pa m³ mol⁻¹ (calc.)

S.g./density 1.622 (20 °C) **Solubility** In water 335 ± 31.5 g/l of solution (or 414 ± 51.8 g/l of water) (pH 4.2, 20 °C). **Stability** Stable over 5 days at 50 °C (pH 4, 7 and 9).

glyphosate-trimesium

Mol. wt. 245.2 **M.f.** $C_6H_{16}NO_5PS$ **Form** White solid. **M.p.** Decomp. 150 °C **V.p.** <0.01 mPa

(20 °C) **K_{ow}** $\log P = -2.9$ **Henry** $< 2 \times 10^{-9}$ Pa m³ mol⁻¹ (calc.) **S.g./density** 1.42 **Solubility** In

water >1000 g/l. In acetone, chlorobenzene, ethanol, kerosene, xylene <5 (all in g tech./l).

COMMERCIALISATION: **History** Herbicidal activity reported by D. D. Baird et al. (*Proc. North Cent. Weed Control Conf.*, 1971, **26**, 64). The isopropylamine, sodium and ammonium salts introduced by Monsanto Co. in 1974; the trimesium (trimethylsulfonium) salt introduced in Spain (1989) by ICI Agrochemicals (now Syngenta AG). **Patents** US 3799758 (to Monsanto); EP 53871; US 4315765 (both to ICI) **Manufacturers** Agrochem; Aimco; Aragro; Atanor; Atul; Cheminova; Comlets; DongHua; Dow AgroSciences; Drexel; Excel; Feinchemie Schwebda; Hebei Golhil; Herbex; High Kite; ICN Hungary; Makhteshim-Agan; Monsanto; Nortox; Nufarm Ltd; Pyosa; Reposo; Sabero; Sannong; Sharda; Sundat; Syngenta; Xinan.

APPLICATIONS: **Biochemistry** Inhibits 5-enolpyruvylshikimate-3-phosphate synthase (EPSPS), an enzyme of the aromatic acid biosynthetic pathway. This prevents synthesis of essential aromatic amino acids needed for protein biosynthesis. **Mode of action** Non-selective systemic herbicide, absorbed by the foliage, with rapid translocation throughout the plant. Inactivated on contact with soil. **Uses** Control of annual and perennial grasses and broad-leaved weeds, pre-harvest, in cereals, peas, beans, oilseed rape, flax and mustard, at c. 1.5–2 kg/ha; control of annual and perennial grasses and broad-leaved weeds in stubble and post-planting/pre-emergence of many crops; as a directed spray in vines and olives, at up to 4.3 kg/ha; in orchards, pasture, forestry and industrial weed control, at up to 4.3 kg/ha. As an aquatic herbicide, at c. 2 kg/ha. **Formulation types** SG; SL. **Compatibility** Mixing with other herbicides may reduce the activity of glyphosate.

glyphosate

Selected products 'Gladiator' (Devidayal); 'Glyphotox' (Aimco); 'Pilarsato' (Pilarquim); 'Rinder' (Inquiport); 'Rophosate' (Rotam); 'Seccherba' (Agrimix); **mixtures** 'Illico' (+ amitrole) (Nufarm SA).

glyphosate-isopropylammonium

Selected products 'Roundup' (Monsanto); 'Sting' (Monsanto); 'Asset' (Ancom); 'Cosmic' (Calliope); 'Gallup' (Barclay); 'Glistar' (ICN Hungary); 'Glycel' (Excel); 'Glyphogan' (Makhteshim-Agan); 'Glyphomax Plus' (Dow AgroSciences); 'Ground-Up' (Vapco); 'Nufosate' (Nufarm UK); 'Oxalis' (Calliope); 'Rodeo' (Dow AgroSciences); 'Rondo' (Reposo); 'Sanos' (Sanonda); 'Taifun' (Feinchemie Schwebda); 'Vifosat' (Vipesco); 'Yerbimat' (Ingeniería Industrial); **mixtures** 'Oriflam' (+ amitrole) (Nufarm SA); 'Rebin GT' (+ butafenacil) (Syngenta).

glyphosate-trimesium

Selected products 'Touchdown' (Syngenta).

ANALYSIS: **Product** analysis by hplc with u.v. detection (AOAC Methods, 17th Ed., 983.10; CIPAC Handbook, 1985, 1C, 2132; *ibid.*, 1998, H, 182) or by ion-exchange lc with u.v. detection (AOAC Methods, 17th Ed., 996.12). **Residues** determined by glc (Pestic. Anal. Man., 1979, II), by gc with MSD (also applicable to aminomethylphosphonic acid, AOAC Methods, 17th Ed., 2000.05) or by hplc with o-phthalaldehyde post-column reaction specific for primary amines (J. Agric. Food Chem., 1986, 34(6), 955-960). In **environmental water**, by hplc determination by o-phthalaldehyde post-column reaction system (AOAC Methods, 17th Ed., 991.08, 10.6.18).

MAMMALIAN TOXICOLOGY: *glyphosate*

Reviews FAO/WHO 47, 49, 80, 82 (see part 2 of the Bibliography). **Oral** Acute oral LD₅₀ for rats 5600, mice 11 300, goats 3530 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >5000 mg/kg. Eye irritant; non-irritating to skin (rabbits). **Inhalation** LC₅₀ (4 h) for rats >4.98 mg/l air. **NOEL** In 2 y feeding trials, no ill-effects were observed in rats receiving 410 mg/kg diet daily (average) and, in 1 y feeding trials, no ill-effects were observed in dogs receiving 500 mg/kg daily (highest dose treated). Lowest relevant NOAEL (2 y) for rats 31 mg/kg b.w. daily (EU). **ADI** (JMPR) 0.3 mg/kg b.w. [1986, 1997] (for sum of glyphosate and its metabolite AMPA). **Water GV** Unnecessary to recommend a guideline value because not hazardous to health at concentrations normally found in drinking water. **Other** Not mutagenic, not carcinogenic, not teratogenic, not neurotoxic. No adverse effects on reproduction. **Toxicity class** WHO (a.i.) U; EPA (formulation) III **EC classification** Xi; R41| N; R51, R53

glyphosate-ammonium

Oral Acute oral LD₅₀ for rats 4613 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >5000 mg/kg. Slight eye irritant; not a skin irritant (rabbits). **Inhalation** LC₅₀ for rats (whole body) >1.9 mg/l air. **ADI** See glyphosate. **Toxicity class** EPA (formulation) III

glyphosate-isopropylammonium

Oral Acute oral LD₅₀ for rats >5000, goats 5700 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >5000 mg/kg. Slight eye irritant; not a skin irritant (rabbits). **Inhalation** LC₅₀ (4 h) for rats >1.3 mg/l air. **NOEL** In a 6 mo capsule trial, no ill-effects were observed in dogs receiving 300 mg/kg daily (highest dose treated). **ADI** See glyphosate. **Toxicity class** EPA (formulation) III

glyphosate-sodium

Skin and eye Acute oral LD₅₀ for rats >5000 mg/kg. Slight eye irritant; not a skin irritant (rabbits). **ADI** See glyphosate.

glyphosate-trimesium

Oral Acute oral LD₅₀ for male rats 748, female rats 755, mice 1250 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >2000 mg/kg. **Inhalation** LC₅₀ (4 h) for rats 6.2 mg/l air. **NOEL** 100 mg/kg daily. No teratogenic effect observed. **ADI** 25 mg/kg b.w. **EC classification** Xn; R22| N; R51, R53

ECOTOXICOLOGY: *glyphosate*

Birds Acute oral LD₅₀ for bobwhite quail >3851 mg/kg. Dietary LC₅₀ (8 d) for quail and ducks >4640 mg/kg diet. **Fish** LC₅₀ (96 h) for trout 86, bluegill sunfish 120, harlequin fish 168, sheepshead minnow >1000 mg/l. **Daphnia** LC₅₀ (48 h) 780 mg/l. **Algae** EC₅₀ (72 h) for *Selenastrum capricornutum* 485 mg/l, (7 d) 13.8 mg/l; (96 h) for *Skeletonema costatum* 1.2 mg/l, (7 d) 0.64 mg/l; (7 d) for *Navicula pelliculosa* 42, *Anabaena flos-aquae* 15 mg/l. **Other aquatic spp.** LC₅₀ (96 h) for mysid shrimps (*Mysidopsis bahia*) >1000, grass shrimps 281,

fiddler crabs 934 mg/l. EC₅₀ (96 h) for sea urchins >1000 mg/l; (14 d) for *Lemna gibba* 25.5 mg/l. EC₅₀ (48 h) for *Litoria moorei* tadpoles 111 mg/l. **Bees** LD₅₀ (contact and oral) >100 µg/bee.

glyphosate-isopropylammonium

Fish LC₅₀ (96 h) for trout and bluegill sunfish >1000, fathead minnow 97, channel catfish 130 mg/l.

Daphnia LC₅₀ (48 h) 930 mg/l. **Algae** EC₅₀ (72 h) for *Scenedesmus subspicatus* 72.9 mg/l.

Other aquatic spp. EC₅₀ (48 h) for midge larvae 5600, *Litoria moorei* tadpoles >343 mg/l.

Worms LC₅₀ (14 d) for *Eisenia foetida* >5000 mg/kg soil. Reproductive toxicity NOEC

28.79 mg/kg. **Other beneficial spp.** No effects on carabid beetles; harmless to slightly harmful to green lacewing, parasite species, mites/spiders and insects, except moderately harmful to *Bembidion lampros* (EU Guidelines).

glyphosate-trimesium

Birds Acute oral LD₅₀ for bobwhite quail >2050, mallard ducks 950 mg tech./kg. **Fish** LC₅₀ (96 h) for trout 1800, bluegill sunfish >3500 mg/l. **Daphnia** LC₅₀ (48 h) 12 mg/l. **Algae** EC₅₀ 19 mg/l.

Bees LD₅₀ (contact) 0.39 mg/bee; (oral) >0.4 mg/bee. **Worms** LD₅₀ (14 d) >1000 mg/kg soil.

Other beneficial spp. Harmless under field conditions at field application rates to parasitic wasps (*Aphidius rhopalosiphi*), lycosid spiders and carabid beetles (*Pterostichus melanarius*).

ENVIRONMENTAL FATE: EHC 159 (WHO, 1994). **Animals** In mammals, following oral administration, glyphosate is very rapidly excreted unchanged and does not bioaccumulate.

Plants Slowly metabolised to aminomethylphosphonic acid ([1066-51-9]), which is the major plant metabolite.

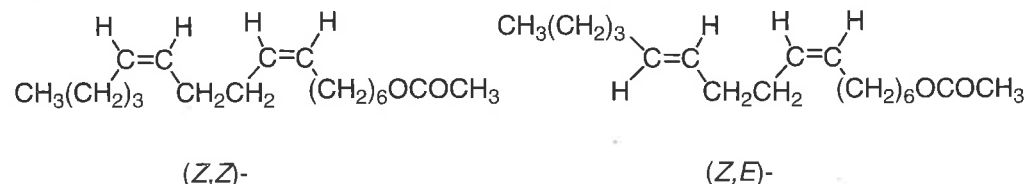
Soil/Environment In soil (field), DT₅₀ 1-130 d, depending on edaphic and climatic conditions. In water, DT₅₀ varies from a few to 91 d. Photodegradation in water occurs under natural conditions, DT₅₀ 33-77 d; no substantial photodegradation in soil was recorded over 31 d. In a lab. whole system with water and sediment, DT₅₀ 27-146 d (aerobic), 14-22 d (anaerobic). The major metabolite in soil and water is aminomethylphosphonic acid.

420 gossyplure

Insect pheromone

See also *The BioPesticide Manual*

pheromone



The mating pheromone of the pink bollworm moth (*Pectinophora gossypiella*).

NOMENCLATURE: IUPAC name a 1:1 mixture of (Z,Z)- and (Z,E)-hexadeca-7,11-dien-1-yl acetate

Chemical Abstracts name a 1:1 mixture of (Z,Z)- and (Z,E)-7,11-hexadecadien-1-ol acetate

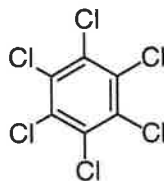
2.2 µg/l. **Algae** EC₅₀ (72 h) 20 mg/l. **Bees** Toxic to bees. **Worms** LC₅₀ (14 d) for *Eisenia foetida* 98 mg/kg dry, artificial soil. **Other beneficial spp.** Harmless to *Chrysoperla* larvae.

ENVIRONMENTAL FATE: EHC 63 (WHO, 1986; a general review of organophosphorus insecticides). **Animals** In rats, following oral administration, 90% is excreted in the urine and 6% in the faeces in metabolised form within 6 days. **Plants** Four days after application to lettuce, the compound is completely metabolised to polar, water-soluble compounds without accumulation of any intermediate. **Soil/Environment** In soil, rapidly degraded by micro-organisms, DT₅₀ (field) 1.4 d, DT₉₀ (field) 4.6 d, depending on temperature and soil type; no accumulation. In lab. (aerobic), DT₅₀ <4 h, DT₉₀ 40 h (20°C). Degradation in water phase of water sediment system is very quick, DT₅₀ 27–77 h.

433 *Heterorhabditis bacteriophora* and *H. megidis* Biological insecticide

Insect parasitic nematodes used for control of Japanese beetles, black vine weevils, etc. For full details, see *The BioPesticide Manual*.

434 hexachlorobenzene Fungicide



NOMENCLATURE: **Common name** hexachlorobenzene (BSI, E-ISO, F-ISO, accepted in lieu of a common name)

IUPAC name hexachlorobenzene

Chemical Abstracts name hexachlorobenzene

Other names HCB **CAS RN** [118–74–1] **EC no.** 204–273–9

PHYSICAL CHEMISTRY: **Mol. wt.** 284.8 **M.f.** C₆Cl₆ **Form** Colourless crystals. **M.p.** 226°C; (tech., ≥220°C) **B.p.** 323–326°C **V.p.** 1.45 mPa (20°C) **S.g./density** 2.044 (23°C)

Solubility Practically insoluble in water. Soluble in hot benzene, chloroform, carbon disulfide, and diethyl ether. Sparingly soluble in carbon tetrachloride. Practically insoluble in cold alcohols.

Stability Very stable to acids and alkalis, even at 85°C and pH 3, 7 and 11 (*Agchem. Desk Ref.*).

COMMERCIALISATION: **History** Fungicidal seed treatment reported by H. Yersin *et al.* (*C. R. Seances Acad. Agric. Fr.*, 1945, **31**, 24).

APPLICATIONS: **Mode of action** Selective fungicide. Acts by fumigant action on fungal spores.

532 hexachlorobenzene

Uses Seed treatment for control of common bunt and dwarf bunt of wheat.

Formulation types DS; WS.

ANALYSIS: **Residues** determined by glc (AOAC Methods, 17th Ed., 977.19, 980.22; *Pestic. Anal. Man.*, 1979, **1**, 201-A, 201-G; *Analyst (London)*, 1979, **104**, 425; A. Ambrus et al., *J. Assoc. Off. Anal. Chem.*, 1981, **64**, 773; *Man. Pestic. Residue Anal.*, 1987, **1**, 1, 5, 6, S9, S10, S12, S19; *Anal. Methods Residues Pestic.*, 1988, Part I, M1, M12). In **drinking water** by glc with ECD (AOAC Methods, 17th Ed., 990.06).

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 30, 31 (see part 2 of the Bibliography). See also WHO Technical Report Series No. 555 (1974); P. Cooper, *Food Cosmet. Toxicol.*, 1976, **14**, 351–353; and W. Hayes & E. Hawes, *Handbook of Pesticide Toxicology*, 1991, **3**, 1422–1433.

IARC ref. 20; Suppl. 7; **class** 2B **Oral** Acute oral LD₅₀ for rats 10 000 mg/kg; guinea pigs tolerated doses >3000 mg/kg. **Skin and eye** May cause slight skin irritation. **ADI** (JMPR) Conditional ADI withdrawn [1978]. **Water GV** 1 µg/l (based on incidence of cancer in animals). **Other** There is evidence that hexachlorobenzene is carcinogenic in mice and hamsters, and may represent a carcinogenic risk to man. Non-mutagenic in *in vitro* and *in vivo* studies, but is foetotoxic and produces some teratogenic effects. Has caused a serious outbreak of porphyria in humans. **Toxicity class** WHO (a.i.) Ia; EPA (formulation) IV **EC classification** R45] T; R48/25] N; R50, R53 **PIC** Yes

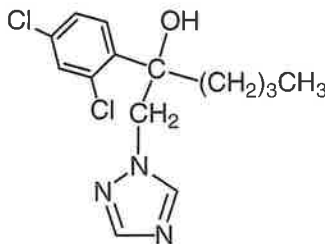
ECOTOXICOLOGY: **Fish** LC₅₀ (96 h) for five freshwater species 0.05–0.2 mg/l. **Bees** Not toxic to bees.

ENVIRONMENTAL FATE: EHC 195 (WHO, 1997). **Animals** The principal metabolites in mammals are pentachlorophenol, tetrachlorohydroquinone and pentachlorothiophenol, with lesser amounts of tetrachlorobenzene, pentachlorobenzene, 2,4,5- and 2,4,6-trichlorophenols and 2,3,4,6- and 2,3,5,6-tetrachlorophenols.

435 hexaconazole

Fungicide

FRAC 3, G1; DMI: triazole



NOMENCLATURE: **Common name** hexaconazole (BSI, ANSI, draft E-ISO, (m) draft F-ISO)

IUPAC name (R_S)-2-(2,4-dichlorophenyl)-1-(1H-1,2,4-triazol-1-yl)hexan-2-ol

Chemical Abstracts name (±)-α-butyl-α-(2,4-dichlorophenyl)-1H-1,2,4-triazole-1-ethanol

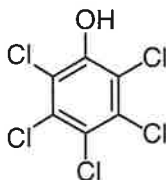
CAS RN [79983–71–4] **Development codes** PP523; ICIA0523 (both ICI)

PHYSICAL CHEMISTRY: **Composition** Tech. is >85% pure. **Mol. wt.** 314.2 **M.f.** C₁₄H₁₇Cl₂N₃O **Form** White crystalline solid. **M.p.** 110–112°C **V.p.** 0.018 mPa (20°C) **K_{ow}** logP = 3.9 (20°C)

hexaconazole 533

623 pentachlorophenol

Insecticide, fungicide, herbicide



NOMENCLATURE: *pentachlorophenol*

Common name PCP (WSSA, JMAF); pentachlorophenol (BSI, E-ISO, F-ISO, accepted in lieu of a common name)

IUPAC name pentachlorophenol

Chemical Abstracts name pentachlorophenol

CAS RN [87-86-5] **EC no.** 201-778-6

sodium pentachlorophenoxide

Common name sodium pentachlorophenoxide (BSI, E-ISO); pentachlorophénate de sodium (F-ISO)

IUPAC name sodium pentachlorophenoxide; sodium pentachlorophenate

CAS RN [131-52-2] **EC no.** 205-025-2

pentachlorophenyl laurate

IUPAC name pentachlorophenyl laurate

Chemical Abstracts name pentachlorophenyl dodecanoate

CAS RN [3772-94-9]

PHYSICAL CHEMISTRY: *pentachlorophenol*

Mol. wt. 266.3 **M.f.** C_6HCl_5O **Form** Colourless crystals, with a phenolic odour; (tech., dark grey). **M.p.** 191°C; (tech., 187–189°C) **B.p.** 309–310°C (decomp.) **V.p.** 16 Pa (100°C)

K_{ow} logP = 5.1 (25°C, unionised) (K. Chamberlain et al., *Pestic. Sci.*, 1996, **47**, 265)

S.g./density 1.98 (22°C) **Solubility** In water 80 mg/l (30°C). Soluble in most organic solvents, e.g. acetone 215 g/l (20°C). Slightly soluble in carbon tetrachloride and paraffins. The sodium, calcium and magnesium salts are soluble in water. **Stability** Relatively stable and non-hygroscopic.

pKa 4.71 **F.p.** Not flammable

sodium pentachlorophenoxide

Mol. wt. 288.3 **M.f.** C_6Cl_5NaO **Solubility** Crystallises from water as a monohydrate, solubility in water 330 g/l (25°C). Insoluble in petroleum oils.

pentachlorophenyl laurate

Mol. wt. 448.6 **M.f.** $C_{18}H_{23}Cl_5O_2$

COMMERCIALISATION: **History** Introduced c. 1936 as a timber preservative and later used as a general disinfectant. **Manufacturers** Excel.

APPLICATIONS: **Mode of action** Insecticide, fungicide, and non-selective contact herbicide.

Uses Pentachlorophenol is used to control termites and, frequently, as an ester (such as pentachlorophenyl laurate), to protect wood from fungal rots and wood-boring insects, and as a general herbicide. The sodium salt is used as a general disinfectant, e.g. for trays in mushroom houses. **Formulation types** GR; OL; WP. **Selected products** 'Biocel Sg 85' (Excel).

pentachlorophenol 755

ANALYSIS: **Product** analysis by titration with alkali (MAFF Ref. Bk., 1958, No. 1, p. 64).

Residues determined by colorimetry of derivatives (W. W. Kilgore & K. W. Cheng, *Anal. Methods Pestic. Plant Growth Regul. Food Addit.*, 1967, **5**, 313; *Anal. Methods Pestic. Plant Growth Regul.*, 1972, **6**, 581) or by glc (AOAC Methods, 17th Ed., 985.24). In **drinking water**, by conversion to methyl ester with diazomethane, then glc with ECD (*ibid.*, 992.32).

MAMMALIAN TOXICOLOGY: *pentachlorophenol*

IARC ref. 53, 71 **Oral** Acute oral LD₅₀ for rats 210 mg/kg. **Skin and eye** Irritating to skin (the solid and aqueous solutions >10 g/l), eyes, and mucous membranes. **NOEL** No deaths occurred among dogs and rats receiving 3.9–10 mg daily for 70–190 d. **Water** GV 9 µg/l (based on incidence of cancer in animals). **Toxicity class** WHO (a.i.) Ib; EPA (formulation) II
EC classification R40| T+; R26| T; R24/25| Xi; R36/37/38| N; R50, R53 (also applies to the sodium salt) **PIC** Yes

ECOTOXICOLOGY: *sodium pentachlorophenoxide*

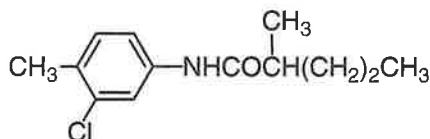
Fish LC₅₀ (48 h) for rainbow and brown trout 0.17 mg/l (J. S. Alabaster, *Proc. Br. Weed Control Conf.*, 4th, 1958, p. 84).

ENVIRONMENTAL FATE: **EH** 71 (WHO, 1987). **Animals** The principal metabolites in female rats were tetrachloromonophenols, diphenols and hydroquinones (G. Renner & C. Hopper, *Xenobiotica*, 1990, **20**, 573). **Soil/Environment** Very persistent in the environment.

624 pentanochlor

Herbicide

HRAC C₂ WSSA 7; anilide



NOMENCLATURE: **Common name** pentanochlor (BSI, E-ISO); pentanochlore ((f) F-ISO); solan (WSSA, Canada, ex ANSI); CMMP (JMAF)

IUPAC name 3'-chloro-2-methylvalero-p-toluidide

Chemical Abstracts name N-(3-chloro-4-methylphenyl)-2-methylpentanamide

CAS RN [2307-68-8] **Development codes** FMC 4512

PHYSICAL CHEMISTRY: **Mol. wt.** 239.7 **M.f.** C₁₃H₁₈ClNO **Form** Colourless solid; (tech., colourless to pale cream powder). **M.p.** 85–86 °C (pure); 82–86 °C (tech.) **V.p.** Very low at room temperature **S.g./density** 1.106 (20 °C) **Solubility** In water 8–9 mg/l (20 °C). In di-isobutyl ketone 460, isophorone 550, methyl isobutyl ketone 520, xylene 200–300, pine oil 410 (all in g/kg, 20 °C). **Stability** Stable to hydrolysis in neutral media at room temperature.

COMMERCIALISATION: **History** Herbicide reported by D. H. Moore (*Proc. Northeast. Weed Control Conf.*, 1960, p. 86). Introduced by FMC Corp. (who no longer manufacture or market it). **Patents** GB 869169; US 3020142

APPLICATIONS: **Biochemistry** Photosynthetic electron transport inhibitor at the photosystem II receptor site. **Mode of action** Selective, contact herbicide with absorption via the leaves.

756 pentanochlor

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats 1196 mg/kg. **Skin and eye** Acute dermal toxicity for rats >2000 mg/kg. Non-irritating to skin and eyes (rabbits). Is a skin sensitiser (guinea pigs). **Inhalation** LC₅₀ (4 h) for rats >4.16 mg/l. **NOEL NOAEL** (90 d) for rats 7.5 mg/kg daily. **Other** Not mutagenic, teratogenic or carcinogenic.

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail 1800 mg/kg. Dietary LC₅₀ for bobwhite quail >5000 ppm. **Fish** LC₅₀ (96 h) for rainbow trout 2.2, bluegill sunfish 6.6 mg/l. **Daphnia** EC₅₀ (48 h) 23 mg/l. **Algae** EC₅₀ (120 h) for *Selenastrum* 5.0 µg/l, *Anabaena* 10 mg/l. **Bees** LD₅₀ (48 h) (oral and contact) >200 µg/bee. **Worms** LC₅₀ (14 d) for earthworms 435 mg/kg.

ENVIRONMENTAL FATE: **Animals** Metabolism is similar to that in plants. **Plants** Metabolism proceeds through glutathione conjugation. No residues were detected in harvested crops. **Soil/Environment** DT₅₀ in water/sediment 5.1–10 d. In soil 5.4–7.7 d (20°C, lab. studies), 4.4–22.0 d (field). Degradation proceeds in a similar manner to that in plants.

628 petroleum oils

Acaricide, insecticide, herbicide, adjuvant

NOMENCLATURE: **Other names** mineral oils; white oils (refined grades); paraffin oils; adjuvant oils; spray oils **CAS RN** [64742–55–8]

PHYSICAL CHEMISTRY: **Composition** They consist largely of aliphatic hydrocarbons, both saturated and unsaturated, the content of the latter being reduced by refinement. Produced by the distillation and refinement of crude mineral oils, those used as pesticides generally distil >310°C. They may be classified by the proportion distilling at 335°C, namely: 'light' (67–79%), 'medium' (40–49%) and 'heavy' (10–25%). Adjuvant oils are highly refined self-emulsifying oils which form a quick-breaking emulsion, spread quickly and help penetration of the active ingredient into the plant and pest. **B.p.** Fraction distilling above 310°C **S.g./density** 0.65–1.06 (crude oil); 0.78–0.80 (kerosenes); 0.82–0.92 (spray oils)

COMMERCIALISATION: **History** Oils of higher distillation range came into use c. 1922. Later, highly refined oils were introduced as adjuvants to increase the effectiveness of some other pesticides. **Manufacturers** Chevron.

APPLICATIONS: **Mode of action** Acaricide and insecticide with ovicidal activity; contact herbicide; adjuvant for herbicides. **Uses** Control of overwintering forms (particularly winter eggs) of spider mites, aphids, and scale insects on fruit trees (pome fruit, stone fruit, citrus fruit), vines, and some ornamentals; and scale insects and summer eggs of spider mites and other insects on fruit trees (pome fruit, stone fruit, citrus fruit), vines, olives, bananas, some ornamentals, and glasshouse crops. Control of grass and broad-leaved weeds in umbelliferous crops (including carrots, celery, caraway, chervil, coriander, dill, lovage, and parsley), and in tree nurseries. Also used as a surfactant and as an adjuvant to enhance the activity of herbicides. **Phytotoxicity** Some petroleum oils are phytotoxic to plants, and must therefore be used only during the dormant period. **Formulation types** EC; Oil. **Compatibility** Incompatible with sulfur-containing materials. **Selected products** 'Supreme 415' (Amvac); 'Volck' (Valent).

petroleum oils 761

ANALYSIS: **Formulation** analysis is by standard methods (MAFF Ref. Bk., 1958, No. 1, p. 66; CIPAC Handbook, 1970, 1, 582).

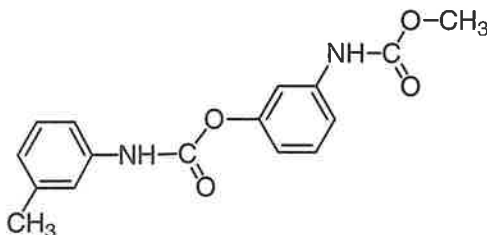
MAMMALIAN TOXICOLOGY: **Skin and eye** Dermal LD₅₀ for rabbits >5000 mg/kg. Not a skin sensitiser (Buehler guinea pig test). **Other** No toxicological problem due to petroleum oils has been reported in practice. **EC classification** Petroleum extracts are classified as R45

ENVIRONMENTAL FATE: **Soil/Environment** No risk of polynuclear aromatic compounds entering the food chain.

629 phenmedipham

Herbicide

HRAC C₁ WSSA 5; phenyl carbamate herbicide



NOMENCLATURE: **Common name** phenmedipham (BSI, E-ISO, ANSI, WSSA, JMAF); phenmédiphame ((*m*) F-ISO)

IUPAC name methyl 3-(3-methylcarbaniloyloxy)carbanilate;

3-methoxycarbonylamino-phenyl 3'-methylcarbanilate

Chemical Abstracts name 3-[(methoxycarbonyl)amino]phenyl (3-methylphenyl)carbamate

Other names PMP **CAS RN** [13684-63-4] **Development codes** SN 38 584 (Schering); ZK 15320; EP-452

PHYSICAL CHEMISTRY: **Composition** Tech. grade is >97% pure. **Mol. wt.** 300.3

M.f. C₁₆H₁₆N₂O₄ **Form** Colourless crystals. **M.p.** 143–144°C; (tech., 140–144°C)

V.p. 1.33 × 10⁻⁶ mPa (25°C) **K_{ow}** logP = 3.59 (pH 3.9) **Henry** 5 × 10⁻⁸ Pa m³ mol⁻¹ (calc.)

S.g./density 0.34–0.54 (20°C) **Solubility** In water 4.7 mg/l (room temperature). Soluble in polar organic solvents. In acetone, cyclohexanone c. 200, methanol c. 50, chloroform 20, benzene 2.5, hexane c. 0.5, dichloromethane 16.7, ethyl acetate 56.3, toluene c. 0.97, 2,2,4-trimethylpentane 1.16 (all in g/l, 20°C). **Stability** Stable up to 200°C. Very stable in acidic media, but hydrolysed in neutral and alkaline media; DT₅₀ (22°C) 50 d (pH 5), 14.5 h (pH 7), 10 min (pH 9). In solution (pH 3.8) irradiated at 280 nm, DT₅₀ 9.7 d. **pKa** <0.1

COMMERCIALISATION: **History** Herbicide reported by F. Arndt & C. Kötter (*Abstr. Int. Congr. Plant Prot.*, 6th, Vienna, 1967, p. 433). Introduced by Schering AG (now Bayer CropScience).

Patents GB 1127050 **Manufacturers** Bayer CropScience; Griffin; Sharda; Synthesia; United Phosphorus Ltd.

APPLICATIONS: **Biochemistry** Photosynthetic electron transport inhibitor at the photosystem II receptor site. **Mode of action** Selective systemic herbicide, absorbed through the leaves, with translocation primarily in the apoplast. **Uses** Used post-emergence, at 1 kg/ha, in beet crops,

762 phenmedipham

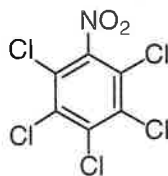
and mallard ducks >5620 mg/kg diet. **Fish** LC₅₀ (96 h) for rainbow trout 0.27, bluegill sunfish >0.28, common carp 0.41 mg/l. **Daphnia** EC₅₀ (48 h) 0.08 mg/l. **Algae** E_bC₅₀ (72 h) 0.058 mg/l. **Other aquatic spp.** NOEC (28 d) for *Chironomus riparius* 0.128 mg/l (water spiked). **Bees** LD₅₀ (oral and contact) >100 µg/bee. **Worms** LC₅₀ (14 d) >923 mg/kg soil. **Other beneficial spp.** Harmless to most non-target arthropod species in laboratory tests (IOBC). Little or no effect in field studies; no effect on soil micro-organisms at 4000 g/ha. See M. Miles & C. Longhurst, *Proc. Br. Crop Prot. Conf. - Pests Dis.*, 2000, **1**, 371.

ENVIRONMENTAL FATE: Slowly biodegraded in plants, animals and soil. However, hydrolysis under acidic conditions, aqueous photolysis, and strong sorption to soils/sediment are important degradation/dissipation processes. Quinoxifen and its residues have negligible leaching potential and will not pose a threat to groundwater. **Animals** Metabolism in goats and hens studied (G. L. Reeves *et al.*, *Proc. Br. Crop Prot. Conf. - Pests Dis.*, 1996, **3**, 1169). **Plants** Only slightly metabolised in wheat, with low residues found in the crop (*idem, ibid.*). Extensively photodegraded on the wheat leaf surface, giving multiple polar degradation products. On grapes and cucumbers grown under glass, the main residue was unchanged quinoxifen. **Soil/Environment** Soil DT₅₀ (field) 11–454 d (biphasic, 10 trials); DT₉₀ (field) >1 y, but does not accumulate under normal practice. DT₅₀ (lab., aerobic) 106–508 d (7 soils, 20–25°C); DT₅₀ (lab. anaerobic) 289 d (20°C). Minimal soil photolysis (est. DT₅₀ (field) >1 y). The main metabolite (3-hydroxyquinoxifen) is formed by hydroxylation of the quinoline ring, and the minor metabolite (5,7-dichloro-4-hydroxyquinoline, DCHQ) is formed by cleavage of the ether bridge, especially in acidic soil. K_{oc} 15 415–75 900; quinoxifen and its residues have no significant leaching potential. **Water** For aqueous hydrolysis in the dark, see Stability. Photolysis in water is more significant, DT₅₀ 1.7 h (June), 22.8 h (December). In dark water/sediment systems, quinoxifen rapidly migrates from water to sediment and is moderately degraded, DT₅₀ (lab.) 35–150 d, to give 3-hydroxyquinoxifen. **Air** No significant volatile losses are expected following application. Any small amounts present in air are estimated to degrade with atmospheric DT₅₀ 1.88 d.

716 quintozene

Fungicide

FRAC 14, F3; aromatic hydrocarbon; chloro/nitrophenyl



NOMENCLATURE: **Common name** quintozene (BSI, E-ISO, (m) F-ISO); PKhNB (USSR); PCNB (JMAF)

IUPAC name pentachloronitrobenzene

Chemical Abstracts name pentachloronitrobenzene

CAS RN [82–68–8] **EC no.** 201–435–0

PHYSICAL CHEMISTRY: **Composition** Tech. grade is 99% pure. **Mol. wt.** 295.3 **M.f.** C₆Cl₅NO₂

Form Colourless needles; (tech., pale yellow crystals). **M.p.** 143–144°C; (tech., 142–145°C)

B.p. 328°C (with slight decomposition) **V.p.** 12.7 mPa (25°C) **K_{ow} logP** = 5.1

quintozene 873

S.g./density 1907 kg/m³ (21°C) **Solubility** In water 0.1 mg/l (20°C). In toluene 1140, methanol 20, heptane 30 (all in g/l). **Stability** Stable to heat. Stable in acidic media, but hydrolysed by alkalis. Some surface colouring after 10 h exposure to sunlight.

COMMERCIALISATION: **History** Introduced as a fungicide by I. G. Farbenindustrie AG (now Bayer AG, who no longer manufacture or market it). **Patents** DE 682048 **Manufacturers** Amvac; Bayer CropScience; Crompton; Mitsui.

APPLICATIONS: **Biochemistry** Proposed mode of action is lipid peroxidation.

Mode of action Seed and soil, contact fungicide. **Uses** Control of damping-off diseases in brassicas, lettuce, cotton, flower crops, tomatoes, etc.; *Rhizoctonia* spp. in brassicas, lettuce, tomatoes and flower crops; bulb rot and tulip fire in tulips; dollar spot, red thread and snow mould in turf; *Rhizoctonia solani* and scab in potatoes; bunt and dwarf bunt of wheat; smut and white rot in onions; white rot in garlic; club root of brassicas; and soil-borne *Sclerotium*, *Sclerotinia* and *Botrytis* spp. in many glasshouse crops. Also used on peanuts, bananas, beans, peas, rice, maize, safflowers, sorghum, soya beans, etc. Applied at 1–1.5 kg/ha. **Formulation types** DP; EC; GR; SC; WP; Seed treatment. **Compatibility** Incompatible with alkaline materials. **Selected products** 'Blocker' (Amvac); 'Folosan' (Crompton); 'RTU' (Gustafson); 'Terraclor' (Crompton); **mixtures** 'System 3' (+ *Bacillus subtilis* + metalaxyl) (Crompton, Helena).

ANALYSIS: **Product** analysis by glc with FID (*CIPAC Handbook*, 1985, **1C**, 2213; *AOAC Methods*, 17th Ed., 982.04). **Residues** determined by glc (*Pestic. Anal. Man.*, 1979, **I**, 201A, 201G, 201I; *Man. Pestic. Residue Anal.*, 1987, **I**, 4–6, S8, S9, S12, S19; *Anal. Methods Residues Pestic.*, 1988, Part I, M1, M12).

MAMMALIAN TOXICOLOGY: **Reviews** FAO/WHO 74, 76 (see part 2 of the Bibliography). Monograph for the placement of quintozone onto Annex 1 of European Directive 91/414 (1997).

IARC ref. 5 **Oral** Acute oral LD₅₀ for rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits >5000 mg/kg. Not irritating to skin; slightly irritating to eyes (rabbits).

Inhalation LC₅₀ (4 h) for rats >1.7 mg/l. **NOEL** (2 y, oncogenic) for rats 1 mg/kg b.w. daily; (1 y, feeding) for dogs 3.75 mg/kg b.w. daily. **ADI** (JMPR) 0.01 mg/kg b.w. (for quintozone containing <0.1% hexachlorobenzene) [1995]. **Toxicity class** WHO (a.i.) U; EPA (formulation) III **EC classification** Xi; R43

ECOTOXICOLOGY: **Birds** LD₅₀ for mallard ducks 2000 mg/kg. Dietary LC₅₀ (8 d) for mallard ducks and bobwhite quail >5000 ppm. **Fish** LC₅₀ (96 h) for rainbow trout 0.55, bluegill sunfish 0.1 ppm. **Daphnia** LC₅₀ (48 h) 0.77 mg/l. **Other aquatic spp.** LC₅₀ (96 h) for shrimps 0.012, oysters 0.029 ppm. **Bees** LD₅₀ (contact) >100 µg/bee.

ENVIRONMENTAL FATE: EHC 41 (WHO, 1984). **Animals** In mammals, the major routes of elimination are as unchanged material in the faeces or as metabolites in the urine. In rats, sheep and monkeys, the principal metabolite is pentachloroaniline (formed by reduction of the nitro group). Other metabolites include pentachlorophenol, pentachlorothioanisole, pentachlorobenzene, bis-methyl-tetrachlorobenzene, methyl pentachlorophenyl sulfide and *N*-acetyl-S-pentachloro=phenylcysteine (E. J. Kuchar et al., *J. Agric. Food Chem.*, 1969, **17**, 1237–1240; W. Koegel et al., *Chemosphere*, 1979, pp. 89–105; P. W. Aschbacher & V. J. Feil, *J. Agric. Food Chem.*, 1983, **31**, 1150). **Plants** In plants, quintozone undergoes conversion to pentachloroaniline, methylthiopentachlorobenzene and a variety of chlorophenyl methyl sulfoxides and sulfones. **Soil/Environment** Persists in soil, with DT₅₀ c. 4–10 mo. Part is lost from the soil by volatilisation. Biodegradation occurs, mainly to pentachloroaniline and also methylthiopentachlorobenzene. For details of effects on soil organisms, see E. R. Ingham, *Crop Prot.*, 1985, **4**, 3–32. K_{oc} for adsorption 6030 (silt loam), 2966 (sand); for desorption 9584 (silt loam), 3285 (sand).

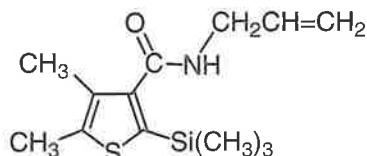
MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for male and female rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for male and female rats >5000 mg/kg. **Inhalation** LC₅₀ (4 h) for rats >6.61 mg/l air. **Other** Non-teratogenic and non-mutagenic.

ECOTOXICOLOGY: **Birds** Acute LD₅₀ for Japanese quail and mallard ducks >2000 mg/kg. **Fish** LC₅₀ (96 h) for carp and rainbow trout >1000 mg/l. **Daphnia** LC₅₀ (3 h) 7.7 mg/l; (24 h) 1.7 mg/l (both Japanese guidelines). **Bees** Oral LD₅₀ (24 h) 0.5 µg/bee (lab. test). **Worms** LD₅₀ for earthworms >1000 mg/kg.

729 silthiofam

Fungicide

FRAC U2, C7; thiophenecarboxamide



NOMENCLATURE: **Common name** silthiofam (BSI, pa ISO)
IUPAC name *N*-allyl-4,5-dimethyl-2-(trimethylsilyl)thiophene-3-carboxamide
Chemical Abstracts name 4,5-dimethyl-*N*-2-propenyl-2-(trimethylsilyl)-3-thiophenecarboxamide
Other names silthiopham **CAS RN** [175217-20-6]
Development codes MON65500 (Monsanto)

PHYSICAL CHEMISTRY: **Mol. wt.** 267.5 **M.f.** C₁₃H₂₁NOSSi **Form** White crystalline powder. **M.p.** 86.1–88.3 °C **K_{ow}** logP = 3.48 (20 °C) **Solubility** In water 35.3 mg/l (20 °C).

COMMERCIALISATION: **History** Discovered in 1993–94 by Monsanto Co. Reported by R. E. Beale et al. (*Proc. Br. Crop Prot. Conf. - Pests Dis.*, 1998, **2**, 343). Introduced in Ireland in 1999. **Patents** EP 538231 **Manufacturers** Monsanto.

APPLICATIONS: **Biochemistry** Inhibits transport of ATP from within the mitochondria to the cytosol (T. Joseph-Horne et al., *Pestic. Biochem. Physiol.*, 2000, **67**, 168). **Mode of action** Protectant fungicide with long-lasting control. **Uses** For antifungal seed treatment in cereals (wheat, barley and triticale). Applied at 25 g/100 kg seed. **Formulation types** FS. **Selected products** 'Latitude' (Monsanto).

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats >5000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >5000 mg/kg. Non-irritating to skin and eyes (rabbits). **Other** Negative in Ames, CHO/HGPRT gene mutation, *in vitro* cytogenicity and mouse micronucleus tests.

ENVIRONMENTAL FATE: **Soil/Environment** In soil, DT₅₀ <365 d.

ANALYSIS: **Product** analysis by glc with TCD (CIPAC Handbook, 1998, H, 255); details from Bayer CropScience. **Residues** determined by glc (G. Dräger, *Pflanzenschutz-Nachr. (Engl. Ed.)*, 1968, 21, 359; *Anal. Methods Pestic. Plant Growth Regul.*, 1972, 6, 483). Methods for the determination of residues are available from Bayer CropScience.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats c. 10 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ (7 d) for rats 65 mg/kg; (4 h) for rats 262 mg/kg. Not irritating to eyes and skin (rabbits). **Inhalation** LC₅₀ (4 h) for rats c. 0.05 mg/l air (aerosol). **NOEL** (2 y) for rats 10, mice 50 mg/kg diet; (13 w) for dogs 0.5 mg/kg diet. **ADI** (BGA) 0.001 mg/kg b.w.

Toxicity class WHO (a.i.) Ia; EPA (formulation) I **EC classification** T+; R27/28

ECOTOXICOLOGY: **Birds** No data; only used as a glasshouse fumigant. **Fish** LC₅₀ (96 h) for golden orfe 0.071, rainbow trout 0.00361 mg/l. **Daphnia** LC₅₀ (48 h) 0.002 mg/l. **Algae** ErC₅₀ for *Scenedesmus subspicatus* 7.2 mg/l. **Bees** No data; only used as a glasshouse fumigant.

ENVIRONMENTAL FATE: **EHC** 63 (WHO, 1986; a general review of organophosphorus insecticides). **Animals** Orally administered sulfotep was absorbed relatively quickly by rats. Elimination took place quickly via the kidney. The main elimination product is the diethylthiophosphate. **Plants** Major metabolites are monothiotep, tetraethylpyrophosphate, diethylthiophosphoric acid and diethylphosphoric acid. **Soil/Environment** K_{oc} value and leaching studies indicate that sulfotep can be classified as immobile. Degraded quickly in different soils. Monothiotep and tetraethylpyrophosphate were very short-lived intermediate products which were degraded to simple thiophosphates or phosphates. In aqueous buffer solutions, sulfotep underwent hydrolysis at environmentally relevant pH levels and temperatures. A direct (primary) photochemical degradation in water could not be ascertained. Low tendency to volatilise.

754 sulfur

Fungicide, acaricide

FRAC M2; multi-site: inorganic

NOMENCLATURE: **Common name** sulfur (E-ISO, JMAF, ESA, accepted in lieu of a common name); soufre (F-ISO, accepted in lieu of a common name)

IUPAC name sulfur

Chemical Abstracts name sulfur

Other names sulphur **CAS RN** [7704-34-9] **EC no.** 231-722-6

Development codes BAS 175 01F (BASF); SAN 7116 (Sandoz)

PHYSICAL CHEMISTRY: **Mol. wt.** 32.1 **M.f.** S_x **Form** Yellow powder, which can exist as various allotropic forms. **M.p.** 114.5°C; (rhombic 112.8°C; monoclinic 119°C) **B.p.** 444.6°C

V.p. 0.527 mPa (30.4°C) (rhombic); 8.6 mPa (59.4°C) **S.g./density** 2.07 (rhombic)

Solubility Practically insoluble in water. Crystalline forms are soluble in carbon disulfide, but amorphous forms are not. Very slightly soluble in ether and petroleum ether; more readily soluble in hot benzene and acetone.

COMMERCIALISATION: **History** Has been used as a pesticide for many years.

Manufacturers Agrochem; Aimco; BASF; Cerexagri; Crystal; Drexel; Excel; FMC; Sharda; Syngenta.

APPLICATIONS: **Biochemistry** Non-specific thiol reactant, inhibiting respiration.

Mode of action Non-systemic protective fungicide with contact and vapour action. Secondary

916 sulfur

acaricidal activity. **Uses** Control of scab on apples, pears, and peaches; powdery mildews on a range of crops, including fruit (at 1.75–6.25 kg/ha), vines (4–10 kg/ha), hops (1.75–6.25 kg/ha), beet (6 kg/ha), cereals (8 kg/ha), citrus (c. 6 kg/ha), ornamentals, cucumbers, vegetables, and in forestry (1.2 kg/ha); shot-hole of stone fruit; and acarinoses of vines. Also controls mites (particularly eriophyid mites) on a range of crops. **Phytotoxicity** Phytotoxic, to some extent, to a number of crops, including cucurbits, apricots, raspberries, and certain other 'sulfur-shy' varieties. **Formulation types** DP; MG; SC; WG; WP. **Compatibility** For reasons of phytotoxicity, mixing with oils should be avoided. **Selected products** 'Cosan' (Bayer CropScience); 'Gold' (Devidayal); 'Kumulus DF' (Micro Flo); 'Lucaflow' (Inquiport); 'Microthiol Special' (Cerexagri); 'Rasulf' (Ramcides); 'Sulfex' (Excel); 'Sulphotox' (Aimco); 'That' (Stoller); 'Thiovit' (Syngenta); **mixtures** 'Kumulan' (+ nitrothal-isopropyl) (BASF); 'Top-Cop' (+ copper sulfate (tribasic)) (Stoller); 'Vizines' (+ zineb) (Vipesco).

ANALYSIS: **Product** analysis is by conversion to sodium thiosulfate which is determined by titration (CIPAC Handbook, 1992, E, 202–210; FAO Plant Prot. Bull., 1961, 9(5), 80). **Residues** may be determined by colorimetry (H. A. Ory et al., Analyst (London), 1957, 82, 189).

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats >5000 mg/kg.

Skin and eye Irritating to skin, eyes, and mucous membranes (not observed with 'Kumulus DF', 'Thiovit Jet'). **Other** Practically non-toxic to humans and animals. **Toxicity class** WHO (a.i.) U; EPA (formulation) IV

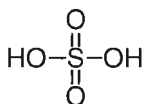
ECOTOXICOLOGY: **Birds** Acute oral LC₅₀ (8 d) for bobwhite quail >5000 ppm. **Fish** Non-toxic to fish. **Daphnia** LC₅₀ (48 h, static) >665 mg/l. **Algae** EC₅₀ (72 h) for *Ankistrodesmus bibraianus* >232 mg/l. **Bees** Non-toxic to bees. **Worms** LC₅₀ (14 d) >1600 mg/l.

Other beneficial spp. Non-toxic to *Coccinella septempunctata*, *Amblyseius potentilla*, *Amblyseius finlandicus*, *Anthocoris nemorum*, *Chrysoperla carnea*. Toxic to *Typhlodromus pyri*, *Trichogramma cacoeciae*, *Coccylornimus turionellae*.

ENVIRONMENTAL FATE: **Plants** Degradation proceeds primarily by microbial reduction in and on plants. **Soil/Environment** Insoluble in water, no leaching potential into groundwater. When oxidised to sulfate, its contribution as sulfate ions from pesticidal sources is negligible in comparison with the natural occurrence of sulfates in soil and water.

755 sulfuric acid

Herbicide



NOMENCLATURE: **Common name** sulfuric acid (E-ISO, accepted in lieu of a common name); acide sulfurique (F-ISO)

IUPAC name sulfuric acid

Chemical Abstracts name sulfuric acid

Other names brown oil of vitriol*; BOV* (for commercial grade) **CAS RN** [7664–93–9]

EC no. 231–639–5

PHYSICAL CHEMISTRY: **Mol. wt.** 98.08 **M.f.** H₂O₄S **Form** Pure sulfuric acid is a colourless,

sulfuric acid 917

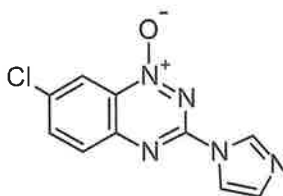
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for Japanese quail 4.2–27.1 mg/kg, depending on carrier and sex. LC₅₀ (8 d) for mallard ducks 325 mg/kg diet. **Fish** LC₅₀ (96 h) for carp 5.6, golden orfe 7.5–18 mg/l. LC₅₀ (21 d) for trout 0.01 mg/l. **Daphnia** LC₅₀ (48 h) 0.003 mg/l. **Algae** LC₅₀ (96 h) 1.15 mg/l. **Bees** Toxic to honeybees. **Worms** LC₅₀ (14 d) for *Eisenia foetida* 187 mg/kg dry artificial soil.

ENVIRONMENTAL FATE: **EHC** 63 (WHO, 1986; a general review of organophosphorus insecticides). **Animals** Mainly eliminated via urine (75–94% of applied radioactivity). Excretion DT₅₀ <1 d. **Plants** In cotton plants, 1-phenyl-3-hydroxy-1,2,4-triazole is found as a metabolite, and the occurrence of a desethyl derivative of triazophos is presumed (W. G. Thier et al., *Fresenius' Z. Anal. Chem.*, 1973, **267**, 181–186). **Soil/Environment** Soil: DT₅₀ (aerobic, field) 6–12 d, DT₉₀ 39–114 d. DT₅₀ (lab.) 7–46 d, DT₉₀ 109–181 d. Water: rapidly degraded in aquatic systems: DT₅₀ (elimination from water) <3 d, (elimination from water/sediment system) <11 d; DT₉₀ (elimination from the system) <47 d.

821 triazoxide

Fungicide

FRAC 35; benzotriazine



NOMENCLATURE: **Common name** triazoxide (BSI, E-ISO, (m) F-ISO)

IUPAC name 7-chloro-3-(1H-imidazol-1-yl)-1,2,4-benzotriazine 1-oxide

Chemical Abstracts name 7-chloro-3-(1H-imidazol-1-yl)-1,2,4-benzotriazine 1-oxide

CAS RN [72459–58–6] **EC no.** 276–668–4 **Development codes** SAS 9244 (Bayer)

PHYSICAL CHEMISTRY: **Mol. wt.** 247.6 **M.f.** C₁₀H₆ClN₅O **Form** Light yellow crystals; (tech., yellow-green crystals). **M.p.** 182°C **V.p.** 1 × 10^{–4} mPa (20°C); 3 × 10^{–4} mPa (25°C)

K_{ow} logP = 2.04 (23°C) **Henry** 7.3 × 10^{–7} Pa m³ mol^{–1} (20°C)

S.g./density 1.577 g/cm³ (22.5°C) **Solubility** In water 34 (pH 7 and 9), 58 (pH 4) (both in mg/l, 20°C). In hexane 0.05, dichloromethane 32, isopropanol 1.8, toluene 6.9 (all in g/l, 20°C).

Stability Photolytically decomposed; DT₅₀ (solid state) 1 d, (dissolved in water) 85 solar h.

Hydrolytic stability depends strongly on pH and temperature; DT₅₀ (extrapolated) 5.8–1380 d (pH 9 – pH 4, 50°C); 7–495 d (pH 9 – pH 7, 25°C).

COMMERCIALISATION: **History** Fungicide evaluated by Bayer AG and first marketed in 1990.

Manufacturers Bayer CropScience.

APPLICATIONS: **Mode of action** Specific non-systemic fungicide. **Uses** Exclusively used as a seed dressing for control of seed-borne *Pyrenophora graminea* and *Pyrenophora teres* in barley. Only used in combination with other fungicides, at a rate of 2–3 g/dt seed. **Phytotoxicity** Shows good seed tolerance at recommended doses. **Formulation types** FS; WS. **Selected products mixtures** 'Raxil S' (+ tebuconazole) (seed treatment) (Bayer CropScience).

triazoxide 995

ANALYSIS: Standard method for **residues** in soil, water, and plants is Bayer method No. 00055 (RA-662/253B), by R. Brennecke: HPLC method for the determination of SAS 9244 residues in soil and water, issued July 24, 1984, and adapted to plant materials by supplement No. E001 (MR-408/95), issued June 1, 1995. Details available from Bayer CropScience.

MAMMALIAN TOXICOLOGY: **Oral** Acute oral LD₅₀ for rats c. 150 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >5000 mg/kg. Non-irritant to skin and eyes (rabbits). **Inhalation** LC₅₀ (4 h) for rats c. 0.75 mg/l (dust). **NOEL** (2 y) for rats 1 mg/kg diet, for mice 5 mg/kg diet; (1 y) for dogs 10 mg/kg diet. **ADI** (Germany, and also Bayer proposed) 0.0005 mg/kg b.w. **Toxicity class** WHO (a.i.) II (company classification)

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for Japanese quail 90 mg/kg. Dietary LC₅₀ (5 d) for Japanese quail 3762, mallard ducklings 850 mg/kg diet. **Fish** LC₅₀ (96 h) for rainbow trout 3.54 mg/l. **Daphnia** LC₅₀ (48 h, static) 7.2 mg/l. **Algae** ErC₅₀ for *Scenedesmus subspicatus* 74 µg/l. **Bees** LD₅₀ (oral) >225 µg/bee; (contact) >200 µg/bee. **Worms** LC₅₀ for *Eisenia foetida* >1000 mg/kg dry soil. **Other beneficial spp.** No effect on soil micro-organisms at 80 g/ha.

ENVIRONMENTAL FATE: **Animals** A complete absorption of triazoxide is followed by fast distribution in the body and rapid elimination; almost 100% of the dose is excreted within 48 hours in the urine and faeces. Extensive metabolism of triazoxide was observed in the animal body (rats).

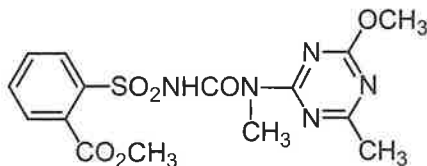
Plants Because of its non-systemic properties, the amount of triazoxide taken up by plants after seed treatment is very low. Residues in the upper plant parts were never found.

Soil/Environment Field studies in Germany revealed a medium fast dissipation rate from soil (average DT₅₀ c. 2 mo). Low application rate (only 2–3 g a.i./dt seed) and low mobility in soil excludes groundwater contamination through leaching. Triazoxide was found to degrade rapidly in natural water/sediment systems, to which aqueous photolysis greatly contributes (environmental DT₅₀ 2.2, 1.7, 4.7, and 9.7 d (calc.) for spring, summer, autumn, and winter, resp.). The use of triazoxide exclusively for seed dressing also minimises exposure in the environment.

822 tribenuron-methyl

Herbicide

HRAC B WSSA 2; sulfonylurea



NOMENCLATURE: *tribenuron-methyl*

Common name tribenuron-methyl

IUPAC name methyl 2-[4-methoxy-6-methyl-1,3,5-triazin-2-yl(methyl)carbamoylsulfonyl]=benzoate

Chemical Abstracts name methyl 2-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)methylamino]=carbonyl]amino]sulfonyl]benzoate

CAS RN [101200-48-0] **EC no.** 401-190-1 **Development codes** DPX-L5300 (DuPont); L5300

996 *tribenuron-methyl*

APPLICATIONS: **Biochemistry** Cholinesterase inhibitor; activity may be due to *in vivo* conversion to dichlorvos (*q.v.*). **Mode of action** Non-systemic insecticide with contact and stomach action.

Uses Insecticidal control in agriculture, horticulture, forestry, food storage, gardening, households, and animal husbandry. In particular, control of Diptera, Lepidoptera, Hymenoptera, Hemiptera and Coleoptera on many crops. For agricultural uses, applied at 300–1200 g/ha. Also used to control household pests, such as flies, cockroaches, fleas, bed bugs, silverfish, ants, etc.; as a fly bait in farm buildings and animal houses; and for control of ectoparasites on domestic animals.

Formulation types DP; GB; GR; PO; SC; SL; SP; UL; WP; Coating agent.

Compatibility Incompatible with alkaline materials and oils. **Selected products** 'Cekufon' (Cequisa); 'Danex' (Makhteshim-Agan); 'Denkaphon' (Denka); 'Dipterex' (Bayer CropScience); 'Lucavex' (Lucava); 'Saprofon' (Sanonda).

ANALYSIS: **Product** analysis by polarography (P. A. Giang & R. L. Caswell, *J. Agric. Food Chem.*, 1957, **5**, 753) or by titration of the chloride ion obtained by hydrolysis (*CIPAC Handbook*, 1970, **1**, 684; FAO Specification (CP/51)). **Residues** determined by glc (*Man. Pestic. Residue Anal.*, 1987, **1**, 6, S13, S19; *Anal. Methods Residues Pestic.*, 1988, Part I, M2, M5, M12; A. Ambrus *et al.*, *J. Assoc. Off. Anal. Chem.*, 1981, **64**, 733). Details available from Bayer CropScience.

MAMMALIAN TOXICOLOGY: **Reviews** JECFA 54, FAO/WHO 30, 31 (see part 2 of the Bibliography). **IARC ref.** 30; **class** 3 **Oral** Acute oral LD₅₀ for male and female rats c. 250 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ (24 h) for male and female rats >5000 mg/kg. Not irritating to skin and eyes (rabbits). **Inhalation** LC₅₀ (4 h) for male and female rats >2.3 mg/l air (aerosol). **NOEL** (2 y) for rats 100, for mice 300 mg/kg diet; (4 y) for dogs 50 mg/kg diet. **ADI** (JECFA) 0.02 mg/kg b.w. [2000]; (JMPR) 0.01 mg/kg b.w. [1978]. **Toxicity class** WHO (a.i.) II; EPA (formulation) II **EC classification** Xn; R22| R43

ECOTOXICOLOGY: **Fish** LC₅₀ (96 h) for rainbow trout 0.7, golden orfe 0.52 mg/l. **Daphnia** LC₅₀ (48 h) 0.00096 mg/l. **Algae** ErC₅₀ for *Scenedesmus subspicatus* >10 mg/l. **Bees** Low toxicity to bees and other beneficial insects.

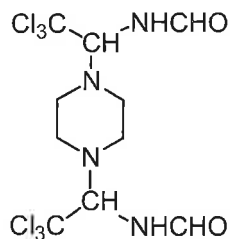
ENVIRONMENTAL FATE: **EHC** 132 (WHO, 1992); 63 (WHO, 1986; a general review of organophosphorus insecticides). EHC 132 notes that trichlorfon is moderately toxic to fish and birds, and moderately to highly toxic to aquatic arthropods, and concludes it should not be sprayed over areas of water. **Animals** In animals, trichlorfon is rapidly absorbed and metabolised. Excretion of the radioactivity in the urine is more or less complete within 6 hours. The major metabolites are dimethylphosphoric acid, monomethylphosphoric acid and conjugates of dichloroacetic acid. **Plants** In plants, trichlorfon is rapidly hydrolysed. The main metabolites are dimethylphosphoric acid and monomethylphosphoric acid and conjugates of dichloroacetic acid and dichloroethanol. **Soil/Environment** Trichlorfon has a relatively high mobility in soil, but it is rapidly metabolised to CO₂. Intermediates are dichloroethanol, dichloroacetic acid and trichloroacetic acid. K_{oc} 20 (±10).

825 *Trichoderma* spp. Biological fungicide

Mitosporic fungi used for control of a range of soil and foliar pathogens. For full details, see *The BioPesticide Manual*.

1000 *Trichoderma* spp.

FRAC 3, G1; DMI: piperazine

**NOMENCLATURE:** Common name triforine (BSI, E-ISO, (f) F-ISO, ANSI, JMAF)IUPAC name *N,N'*-[piperazine-1,4-diylbis[(trichloromethyl)methylene]]diforamamide;1,1'-piperazine-1,4-diyl-di-[*N*-(2,2,2-trichloroethyl)formamide]Chemical Abstracts name *N,N'*-[1,4-piperazinediylbis(2,2,2-trichloroethylidene)]bisformamide

CAS RN [26644-46-2] Development codes Cela W524 (Cela GmbH)

PHYSICAL CHEMISTRY: Mol. wt. 435.0 M.f. C₁₀H₁₄Cl₆N₄O₂ Form White to light brown crystals. M.p. 155°C (decomp.) V.p. 8 × 10¹ mPa (25°C) K_{ow} logP = 2.2 (20°C, unstated pH)Henry 2.5 Pa m³ mol⁻¹ S.g./density 1554 kg/m³ (20°C) Solubility In water 9 mg/l (20°C). Indimethylformamide 330, dimethyl sulfoxide 476, *N*-methylpyrrolidone 476, acetone 11, dichloromethane 1, methanol 10 (all in g/l). Also soluble in tetrahydrofuran; slightly soluble in dioxane and cyclohexanone; insoluble in benzene, petroleum ether and cyclohexane.**Stability** Stable ≤180°C. Decomposed in aqueous solution exposed to u.v. or daylight. Decomposed in strongly acidic media (to trichloroacetaldehyde and piperazine salts) and in strongly alkaline media (to chloroform and piperazine); DT₅₀ (pH 5–7, 25°C) 3.5 d. pKa 10.6, strong base**COMMERCIALISATION:** History Fungicide reported by P. Schicks & K. H. Veen (*Proc. Br. Insectic. Fungic. Conf.*, 5th, 1969, 2, 569). Introduced by Cela GmbH (now BASF AG).

Patents DE 1901421 (to Boehringer) Manufacturers BASF.

APPLICATIONS: Biochemistry Ergosterol biosynthesis inhibitor. Mode of action Systemic fungicide with protective, curative and eradicated properties. Penetrates rapidly into leaves, where it inhibits various stages in the development of fungi. Uses Control of powdery mildews on cereals, fruit, vines, hops, ornamentals, cucurbits, and some vegetables; rusts on cereals, fruit, ornamentals, and beans; *Monilia* spp. on stone fruit; *Ascochyta* blight on chrysanthemums; black spot on roses; scab on apples; and fairy rings on turf. Also suppresses tetranychid mite activity. For stone fruit, applied at 0.33 kg/ha. Phytotoxicity Phytotoxic to certain varieties of pear.**Formulation types** EC; WP. **Compatibility** Should not be mixed with wetting agents, spreader-stickers, or other adjuvants. **Selected products** 'Funginex' (BASF); 'Saprol' (BASF).**ANALYSIS:** Product analysis by rplc with u.v. detection (*CIPAC Handbook*, 1998, H, 299).**Residues** determined by glc (R. Darskus & D. Eichler, *Anal. Methods Pestic. Plant Growth Regul.*, 1978, 10, 243). Details available from BASF.**MAMMALIAN TOXICOLOGY:** Reviews FAO/WHO 80, 82 (see part 2 of the Bibliography).**Oral** Acute oral LD₅₀ for rats >16 000, mice >6000, dogs >2000 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rabbits and rats >10 000 mg/kg. **Inhalation** LC₅₀ (1 h) for rats >4.5 mg/l.**NOEL** (2 y) for rats 200 mg/kg diet, for dogs 100 mg/kg diet. **ADI** (JMPR) 0.02 mg/kg b.w.[1997]. **Other** Acute i.p. LD₅₀ for rats >4000 mg/kg. **Toxicity class** WHO (a.i.) U;

EPA (formulation) IV

1016 triforine

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail >5000 mg/kg. Dietary LC₅₀ (5d) for mallard ducks >4640 mg/kg. **Fish** LC₅₀ (96 h) for bluegill sunfish and rainbow trout >1000 mg/l. **Daphnia** LC₅₀ (48 h) 117 mg/l. **Algae** EC₅₀ for *Scenedesmus subspicatus* 380 mg/l. **Bees** 60 g a.i./hl does not pose a hazard. **Worms** Low toxicity to earthworms; LD₅₀ >1000 mg/kg. **Other beneficial spp.** Harmless to beneficial arthropods. "Harmless" to Hymenoptera (*Trichogramma cacoeciae*, *Encarsia formosa*, *Aphidius matricariae*, *Leptomastix dactylopii*, *Phygadeuon trichops* and *Coccygomimus turionellae*), predatory mites (*Phytoseiulus persimilis*, *Amblyseius andersoni* and *Typhlodromus pyri*), Coleoptera (*Coccinella septempunctata* and *Aleochara bilineata*), *Chiracanthium mildei*, *Anthocoris nemoralis*, *Chrysoperla carnea* and *Forficula auricularia*. "Slightly harmful" to adults of the coccinellid *Semiadalia 11-notata* (IOBC).

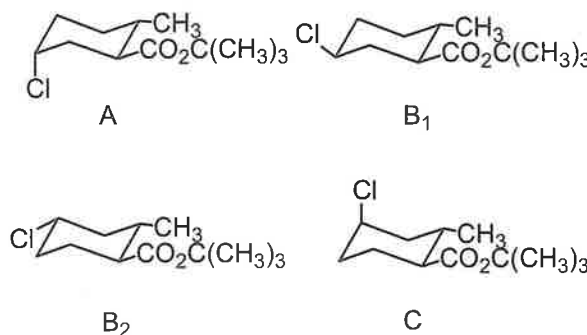
ENVIRONMENTAL FATE: **Animals** In animals, triforine is absorbed rapidly and completely; excretion occurs mainly via the kidney. Triforine and its metabolites show no accumulation ability. **Plants** In barley, beans and tomatoes, after leaf application, triforine is translocated in treated leaves and into newly regrowing plant parts. It is broken down into a large number of polar metabolites in the plant. **Soil/Environment** In soil, a range of non-fungitoxic metabolic end-products is formed, presumably including piperazine (J. P. Rouchard et al., *Pestic. Sci.*, 1978, **9**, 74, 139, 587; A. Fuchs & W. Ost, *Arch. Environ. Contam. Toxicol.*, 1976, **4**, 30–43). DT₅₀ in soil c. 3 w. Soil adsorption Freundlich K 2.75–6.28 in loamy sand and silty loam (o.c. 2.4–6.3%, pH 5.2–7.9). Does not accumulate in the environment.

839 trimedlure

Insect pheromone

See also *The BioPesticide Manual*

synthetic pheromone



Synthetic attractant for male Mediterranean fruit fly (*Ceratitis capitata*).

NOMENCLATURE: **IUPAC name** a mixture of t-butyl 2-methyl-4-chlorocyclohexanecarboxylate and t-butyl 2-methyl-5-chlorocyclohexanecarboxylate stereoisomers

Chemical Abstracts name mixture of 1,1-dimethylethyl 4-chloro-2-methylcyclohexanecarboxylate and 1,1-dimethylethyl 5-chloro-2-methylcyclohexanecarboxylate

Other names TML **CAS RN** [12002–53–8]; [5748–22–1] trimedlure A; [5748–20–9] trimedlure B₁; [5748–21–0] trimedlure B₂; [5748–23–2] trimedlure C

trimedlure 1017

as a mammal and bird repellent. **Phytotoxicity** Non-phytotoxic when used as directed. Phytotoxic to the seeds of some crops, including maize, sorghum, wheat, and rice. **Formulation types** GR; WP.

ANALYSIS: Residues by glc with ECD (S. C. Lau & R. L. Marxmiller, *J. Agric. Food Chem.*, 1970, **18**, 413–415).

MAMMALIAN TOXICOLOGY: Oral Acute oral LD₅₀ for rats 130 mg/kg. Skin and eye Acute percutaneous LD₅₀ for rats >2000 mg/kg. **Toxicity class** WHO (a.i.) O

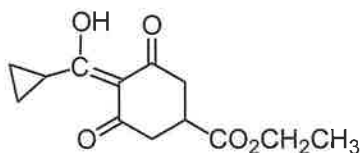
ECOTOXICOLOGY: Fish Toxic to fish. Bees Toxic to bees, in spray formulations.

ENVIRONMENTAL FATE: EHC 64 (WHO, 1986; a review of carbamate insecticides in general).

Animals Metabolism of carbamate insecticides is reviewed (M. Cool & C. K. Jankowski in "Insecticides"). **Plants** In plants, metabolism occurs via hydroxylation of the *N*-methyl group and at the 3- and 4-methyl positions. All metabolites may be conjugated as glucosides.

Soil/Environment Soil DT₅₀ c. 60 d in sterile soil.

841 trinexapac-ethyl *Plant growth regulator*



NOMENCLATURE: *trinexapac-ethyl*

Common name trinexapac-ethyl (BSI, pa E-ISO)

IUPAC name ethyl 4-cyclopropyl(hydroxy)methylene-3,5-dioxocyclohexanecarboxylate

Chemical Abstracts name ethyl 4-(cyclopropylhydroxymethylene)-3,5-dioxocyclohexanecarboxylate

Other names cimectacarb-ethyl* (rejected name) **CAS RN** [95266-40-3]

Development codes CGA 163 935 (Ciba-Geigy)

trinexapac

Common name trinexapac (BSI, pa E-ISO)

CAS RN [104273-73-6] **Development codes** CGA 179500 (Ciba-Geigy)

PHYSICAL CHEMISTRY: *trinexapac-ethyl*

Composition Tech. is ≥92% pure. **Mol. wt.** 252.3 **M.f.** C₁₃H₁₆O₅ **Form** White, odourless solid; (tech. is a yellow to red-brown liquid (30°C) and a solid-liquid melt (20°C), with a slight sweet odour). **M.p.** 36°C **B.p.** >270°C **V.p.** 1.6 mPa (20°C); 2.16 mPa (25°C) (OECD 104)

K_{ow} logP = 1.60 (pH 5.3, 25°C) **Henry** 5.4 × 10⁻⁴ Pa m³ mol⁻¹ **S.g./density** 1.215 g/cm³ (20°C)

Solubility In water 2.8 (pH 4.9), 10.2 (pH 5.5), 21.1 (pH 8.2) (all in g/l, 25°C). In ethanol, acetone, toluene, *n*-octanol 100%, *n*-hexane 5% (25°C). **Stability** Heat-stable up to boiling point.

Photolytically and hydrolytically stable under normal environmental conditions (pH 6–7, 25°C). Less stable in alkali. **pKa** 4.57 **F.p.** 133°C (1013 mbar) (EEC A9)

trinexapac-ethyl 1019

trinexapac

Mol. wt. 224.2 **M.f.** C₁₁H₁₂O₅ **M.p.** 144.4°C **B.p.** c. 220°C **V.p.** 2.3 × 10⁻³ mPa (25°C) (OECD 104, EEC A4) **K_{ow}** logP = 1.8 (pH 2) **S.g./density** 1.41 (20°C) **Solubility** In water 13 (pH 5.0), 200 (pH 6.8), 260 (pH 8.4) (all in g/l). In acetone 95, ethyl acetate 37, methanol 84, octanol 17 (all in g/l). **pKa** pKa₁ 5.32, pKa₂ 3.93

COMMERCIALISATION: **History** First reported by E. Kerber et al. (*Proc. Br. Crop Protection Conf.*, 1989, I, 83). Introduced by Ciba-Geigy AG (now Syngenta AG) and first marketed in Switzerland in 1992. **Patents** EP 126713; US 4693745 **Manufacturers** Syngenta.

APPLICATIONS: *trinexapac-ethyl*

Biochemistry Inhibits 3β-hydroxylation of GA20 to GA3 in gibberellin biosynthesis. The reduced level of gibberellins leads to growth retardation of plants. **Mode of action** Plant growth regulator and retardant, which reduces stem growth by inhibition of internode elongation. Absorbed by the foliage, with translocation to the growing shoot. **Uses** Used for the prevention of lodging in cereals and in winter oilseed rape, at 0.1–0.3 kg/ha. Also used in turf, at 0.15–0.5 kg/ha, to reduce mowing; and as a maturation promoter in sugar cane, at 0.1–0.25 kg/ha. **Phytotoxicity** Could cause inhibition or growth stoppage of some plants, e.g. grasses, aquatic plants and algae.

Formulation types EC; ME; WP. **Compatibility** Compatibility of little importance because of late timing of application; compatible with certain late-season fungicides. **Selected products** 'Bonus' (Syngenta); 'Moddus' (Syngenta); 'Primo' (Syngenta).

ANALYSIS: All methods use hplc, for both ester and acid metabolite.

MAMMALIAN TOXICOLOGY: *trinexapac-ethyl*

Oral Acute oral LD₅₀ for rats 4460 mg/kg. **Skin and eye** Acute percutaneous LD₅₀ for rats >4000 mg/kg. Not irritant to skin or eyes of rabbits. Non-sensitising to skin (guinea pigs). **Inhalation** LC₅₀ (48 h) for rats >5.3 mg/l. **NOEL** (2 y) for rats 115 mg/kg b.w. daily; (18 mo) for mice 451 mg/kg b.w. daily; (1 y) for dogs 31.6 mg/kg b.w. daily. **ADI** 0.316 mg/kg b.w. **Toxicity class** WHO (a.i.) U (company classification)

ECOTOXICOLOGY: *trinexapac-ethyl*

Birds LD₅₀ for ducks and quail >2000 mg/kg. LC₅₀ (8 d) for ducks and quail >5000 ppm.

Fish LC₅₀ (96 h) for trout, carp, bluegill sunfish, catfish, fathead minnow 35–180 mg/l.

Daphnia LC₅₀ (96 h) 142 mg/l. **Bees** Non-toxic; LD₅₀ (oral) >293 µg/bee; (contact) >115 µg/bee. **Worms** Low toxicity to earthworms; LC₅₀ >93 mg/kg.

ENVIRONMENTAL FATE: **Animals** In rats, goats and hens, 90% excretion occurs within 24 hours, all as the acid metabolite. **Plants** Rapid metabolism to the acid, which remains by far the predominant metabolite. **Soil/Environment** In soil, the ester undergoes rapid degradation, DT₅₀ <1 d. The acid has K_d values 1.5–16, K_{oc} 140–600. Further metabolism is rapid, DT₅₀ typically 2–5 w. Within 4–8 w, 50% is mineralised to CO₂.