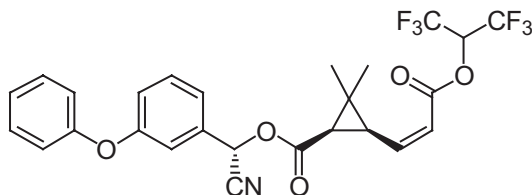


12 acrinathrin

Acaricide, Insecticide

Target Site Sodium channel modulation

IRAC 3A pyrethroid



NOMENCLATURE: **Common name** acrinathrin (BSI, E-ISO); acrinathrine ((f) F-ISO)
IUPAC name (S)- α -cyano-3-phenoxybenzyl (Z)-(1R,3S)-2,2-dimethyl-3-[2-(2,2,2-trifluoro-1-trifluoromethylethoxycarbonyl)vinyl]cyclopropanecarboxylate; *Roth*: (S)- α -cyano-3-phenoxybenzyl (Z)-(1R-cis)-2,2-dimethyl-3-[2-(2,2,2-trifluoro-1-trifluoromethylethoxycarbonyl)vinyl]cyclopropanecarboxylate

Chemical Abstracts name (S)-cyano(3-phenoxyphenyl)methyl (1R,3S)-2,2-dimethyl-3-[(1Z)-3-oxo-3-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]-1-propenyl]cyclopropanecarboxylate

CAS RN [101007-06-1] **EPA PC** 129141 **Development codes** Hoe 076003 (Hoechst); NU 702 (Roussel-Uclaf); RU 38702 (Roussel Uclaf); AE F076003 (AgrEvo)

PHYSICAL CHEMISTRY: **Composition** Tech. is >97% single isomer. **M.f.** C₂₆H₂₁F₆NO₅
Mol. wt. 541.4 **Physical form** White powder (tech.). **M.p. (°C)** 81.5 **V.p. (mPa)** 4.4 × 10⁻⁵ (20 °C) **Henry (Pa m³ mol⁻¹, calc.)** 0.0108 **log K_{ow}** 6.3

Water solubility (mg/l, 20–25 °C) 0.0022 **Organic solubility (g/l, 20–25 °C)** Soluble in acetone (700), 1,2-dichloroethane (650), ethanol (61.4), ethyl acetate (250), hexane (17.5), n-octanol (13), toluene (550), xylene (400) **Specific rotation** [α]_D²⁰ = +17.5°

Hydrolytic stability (DT₅₀) stable (pH 4) (50 °C), 463 d (pH 7), 90.8 h (pH 9) (20 °C)

Aqueous photolytic stability (DT₅₀) 2.3 d

COMMERCIALISATION: **History** Reported by J. R. Tessier *et al.* (*IUPAC Pestic. Chem.*, 1983, **5**, 95). Introduced in France in 1990 by Roussel Uclaf (now Bayer CropScience). Licensed to Cheminova Agro A/S in 2003 then divested to Cheminova (now FMC Corp.) in 2006.

Patents EP 48186; FR 2486073. **Manufacturers** Bayer Vapi; FMC

APPLICATIONS: **Spectrum and Route of Action** Non-systemic acaricide and insecticide active by contact and ingestion. **Uses** Control of phytophagous mites in citrus, top fruit, ornamentals, vegetables, strawberries and vines; control of thrips spp. in tree fruit, vines and vegetables, psyllids in pears, Lepidoptera in pome and stone fruit and leafhoppers in vines, at 20–70 g/ha. **Formulation types** SC; EW; WP; EC **Compatibility** May not be compatible with alkaline products. **Site of Action** Modulation of voltage-gated sodium channels, preventing the channels from closing and resulting in hyperexcitation. **Selected products** Azami Buster (SDS Biotech K.K.); Orytis (FMC); Rufast (FMC)

ANALYSIS: **Product Analysis** HPLC-UV, HPLC-DAD **Residues Analysis (plants, soil, water)** GLC-MS **CIPAC Code** 678

REGULATORY: **Toxicological & Environmental Reviews** EFSA *Jou.*, 2010, **8**, 1872; *ibid.*, 2013, **11**, 3469. **EU status** Approved **Legislation** (EU) 2017/358, (EU) 2019/291, (EU) 540/2011, (EU) 974/2011 **EPA Status** Not Registered **Toxicity class: WHO (a.i.)** U

MAMMALIAN TOXICOLOGY: **Acute oral (LD₅₀, mg/kg)** mice >5000 (tech.) (in corn oil); rats >5000 (tech.) (in corn oil) **Acute dermal (LD₅₀, mg/kg)** rats >2000
Acute Inhalation (LD₅₀, mg/l) rats 1.21 (4 h) **Skin irritation** Not an irritant (rabbits)
Skin sensitisation Not a sensitiser (guinea pigs) **Eye** Not an irritant (rabbits) **NOEL** (90 d) for male rats 2.4 mg/kg b.w. for female rats 3.1 mg/kg b.w.; (1 y) for dogs 3 mg/kg b.w.
 Non-mutagenic and non-teratogenic in rats (2 mg/kg b.w. daily) and rabbits (15 mg/kg b.w. daily).
ADI/RfD (BfR) ADI 0.016 mg/kg b.w. [2006]; (EFSA) ADI 0.01, aRfD 0.01, AOEL 0.007 mg/kg b.w. [2010].

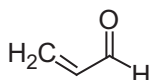
ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail >2250, mallard ducks >2000 mg/kg. Dietary LC₅₀ (8 d) for bobwhite quail 3275, mallard ducks 4175 mg/kg diet.
Fish LC₅₀ for rainbow trout 0.0061, fathead minnows 0.00196, mirror carp 0.12, guppies >0.00492, zebrafish >0.00404 mg/l. **Daphnia** EC₅₀ (48 h) 0.000022 mg/l. **Algae** E_bC₅₀ and E_rC₅₀ (72 h) for *Selenastrum capricornutum* >0.035 mg/l; EC₅₀ (96 h) for *Chlorella vulgaris* >0.82 mg/l. **Bees (LD₅₀, µg/bee)** 0.077 (oral); 0.084 (contact) **Worms** LC₅₀ (14 d) for earthworms >1000 mg/kg soil. **Other beneficial spp.** LR₅₀ (48 h) for *Typhlodromus pyri* 0.006 g/ha.

ENVIRONMENTAL FATE: **Animals** No metabolites found representing >10% of parent compound. **Soil/Environment** Strongly adsorbed onto soil and immobile (irrespective of pH and o.m. content); K_d 2460–2780; K_{oc} 127500–319610. Soil column leaching: <1% of applied acrinathrin found in leachate. DT₅₀ 5–100 d (4 soil types). DT₅₀ under aerobic conditions (pH 6.2, o.m. 3.1%) 52 d. **Plants** The main residue is the parent compound.

13 acrolein

Herbicide

Target Site Multi-site inhibition



NOMENCLATURE: **Common name** acrolein (BSI, ANSI, WSSA, E-ISO, accepted in lieu of a common name); acroléine ((f) F-ISO)

IUPAC name acrylaldehyde; prop-2-enal

Chemical Abstracts name 2-propenal

CAS RN [107-02-8] **EC no.** 203-453-4 **EPA PC** 000701

PHYSICAL CHEMISTRY: **Composition** Tech. is 92–97%. **M.f.** C₃H₄O **Mol. wt.** 56.1

Physical form Colourless mobile liquid with a pungent odour. **M.p. (°C)** –87

V.p. (mPa) 2.9 × 10⁷ (20 °C); 5.9 × 10⁷ (38 °C) **Henry (Pa m³ mol⁻¹, calc.)** 7.8; 19.5 (meas.)

log K_{ow} 1.08 **Water solubility (mg/l, 20–25 °C)** 2.08 × 10⁵

Organic solubility (g/l, 20–25 °C) Soluble in benzene, diethyl ether, ketones, lower alcohols

B.p. 52.5 °C/760 mmHg **F.p.** <–17.8 °C (closed cup) **S.g./Bulk density (20–25 °C)** 0.841

Hydrolytic stability (DT₅₀) 3.5 d (pH 5), 1.5 d (pH 7), 4 h (pH 10) **Thermal stability** stable (<80 °C); reactive chemical; polymerises slowly on storage and violently in presence of concentrated acids, alkalis and amines, may polymerise if exposed to light; must be stored in the dark, under nitrogen.

COMMERCIALISATION: **History** Industrial chemical; introduced as an algicide and aquatic herbicide by Shell Chemical Co. in 1960. Marketed by Baker Petrolite Corporation (now Baker Hughes) since 1962. **Patents** US 2042220; US 2959476. **Manufacturers** Baker Hughes

APPLICATIONS: **Spectrum and Route of Action** Contact herbicide. Breaks down cell walls. **Uses** Control of submersed aquatic weeds and algae in irrigation canals and drainage ditches, at 1–15 mg/l, by injection below the water surface; control of floating weeds, e.g. *Pistia*, *Eichhornia* and *Jussiaea* spp., if concentration is maintained for extended period. **Phytotoxicity** Water for irrigation of crops may be treated at 1–15 ppm. **Formulation types** Liquid **Compatibility** It is not permitted to mix with other preparations. **Site of Action** Chemically reacts, non-specifically, with thiol groups on amino acids and enzymes, resulting in disruption of respiration and other cellular functions. **Selected products** MAGNACIDE H (Baker Hughes)

ANALYSIS: **Residues Analysis (water)** GLC-ECD (*Environ. Chem. Methods*), UV-Vis spectroscopy of the 2,4-dinitrophenylhydrazone, differential pulse polarography

REGULATORY: **Toxicological & Environmental Reviews** EHC 127 (1991); HSG 67 (1991); ICSC 0090 (2001); CICAD 43 (2002); IARC 63 (1995); EPA RED, Sep. 2008.

EPA Status Reregistration **IARC class** 2A **Toxicity class:** WHO (a.i.) Ib

MAMMALIAN TOXICOLOGY: **Acute oral (LD₅₀, mg/kg)** rats 29; mice (female) 17.7; mice (male) 13.9 **Acute dermal (LD₅₀, mg/kg)** rabbits 231 **Acute Inhalation (LD₅₀, mg/l)** rats 8.3 (4 h) **Skin irritation** Irritant **NOEL** (90 d) for rats 5 mg/kg b.w. daily. Administration of 200 mg acrolein/l water to rats for 90 d causes no ill-effects. No reproductive toxicity in 2-generation feeding study in rats at 7.2 mg/kg daily. No teratogenic effect in rabbits at levels causing maternal toxicity (maximum dose 2 mg/kg daily). **ADI/RfD** (EPA) cRfD 0.0005 mg/kg b.w. [2003].

ECOTOXICOLOGY: **Birds** Acute oral LD₅₀ for bobwhite quail 19, mallard ducks 30.2 mg/kg (tech.). **Fish** LC₅₀ (24 h) for rainbow trout 0.15, bluegill sunfish 0.079, shiners 0.04, mosquito fish 0.39 mg/l. **Daphnia** LC₅₀ (48 h) 0.022 mg/l. **Algae** EC₅₀ (120 h) for *Selenastrum capricornutum* 0.050, *Anabaena flos-aquae* 0.042, *Navicula pelliculosa* 0.07, *Skeletonema costatum* 0.03 mg/l. **Other aquatic spp.** LC₅₀ (48 h) for shrimps 0.10, oysters 0.46 mg/l; EC₅₀ (14 d) for *Lemna gibba* 0.07 mg/l.

ENVIRONMENTAL FATE: **Animals** In goat and hen, no acrolein was detected in tissues or excreta, or in goat milk or hen eggs, following administration of high doses. All residues identified are natural products. Data on naturally occurring metabolites found in aquatic species are also available. **Soil/Environment** DT₅₀ in water 150 h (pH 5), 120–180 h (pH 7), 5–40 h (pH 9). Acrolein is metabolised easily in soil, being mineralised to CO₂. In field dissipation studies, DT₅₀ 7.5–10.2 h. Metabolic pathways involving oxidation, reduction and hydration have been proposed. **Plants** Following high application rates to lettuce, no acrolein was detected 1 day following last application. At harvest, 3 highly polar conjugates (representing in total <0.5 ppm) were detected.