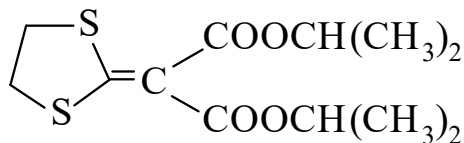




>>Entry Name: Isoprothiolane, BSI, ISO, JMAF

Synonym(s): Bis(1-methylethyl) 1,3-dithiolan-2-ylidenepropanedioate, gCl. Diisopropyl 1,3-dithiolan-2-ylidenemalonate. Fuji-one. IPT



CAS Registry Number: 50512-35-1

Related CAS Registry Numbers(s): 108114-60-9 108114-61-0

Molecular Formula: C₁₂H₁₈O₄S₂

Molecular Weight: 290.404

Accurate Mass: 290.06465

Percentage Composition: C 49.63%; H 6.25%; O 22.04%; S 22.08%

Use/Importance: Agricultural fungicide for rice crops

Physical Description: Cryst.

Melting Point: Mp 50-54.5°

Solubility: V. spar. sol. H₂O

Hazard & Toxicity: LD₅₀ (rat, orl) 1190 mg/kg

>>Derivative: S-Oxide, (±)-

Synonym(s): Isoprothiolane sulfoxide

CAS Registry Number: 52303-69-2

Molecular Formula: C₁₂H₁₈O₅S₂

Molecular Weight: 306.403

Accurate Mass: 306.059565

Percentage Composition: C 47.04%; H 5.92%; O 26.11%; S 20.93%

Physical Description: Needles (hexane/CH₂Cl₂)

Melting Point: Mp 85-86°

>>Derivative: S¹,S³-Dioxide

CAS Registry Number: 133188-15-5

Molecular Formula: C₁₂H₁₈O₆S₂

Molecular Weight: 322.403

Accurate Mass: 322.05448

Percentage Composition: C 44.71%; H 5.63%; O 29.78%; S 19.89%

Physical Description: Yellow needles (hexane/CH₂Cl₂)

Melting Point: Mp 97-100°

References:

Japan. Pat., 1970, 73 33 749; CA, **80**, 120903v

Tsumura, T., *Jpn. Pestic. Inf.*, 1976, **27**, 20, (activity, tox, metab)

Uchida, M. *et al.*, *Agric. Biol. Chem.*, 1985, **49**, 1127, (metab)

Katagiri, N. *et al.*, *Chem. Pharm. Bull.*, 1990, **38**, 3242, (oxides)

Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A947

Pesticide Manual, 11th edn., 1991, No. 432