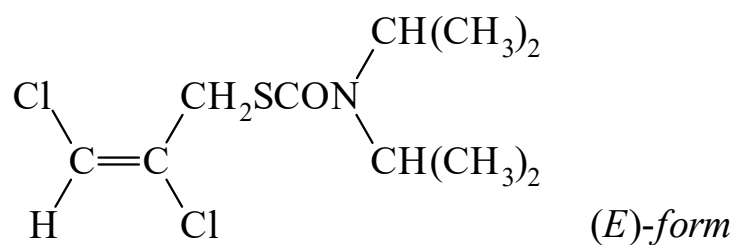




>>Entry Name: Diallylate, BSI

Synonym(s): *S*-(2,3-Dichloro-2-propenyl) bis(1-methylethyl)carbamothioate, 9Cl. *S*-2,3-Dichloroallyl diisopropylthiocarbamate. Avadex



CAS Registry Number: 2303-16-4

Molecular Formula: C₁₀H₁₇Cl₂NOS

Molecular Weight: 270.222

Accurate Mass: 269.040788

Percentage Composition: C 44.45%; H 6.34%; Cl 26.24%; N 5.18%; O 5.92%; S 11.87%

Use/Importance: Herbicide

Boiling Point: Bp₉ 150°

Hazard & Toxicity: LD₅₀ (rat, orl) 395 mg/kg

Supelco: R47-2190

>>Variant: (E)-form

CAS Registry Number: 17708-58-6

Molecular Formula: C₁₀H₁₇Cl₂NOS

Molecular Weight: 270.222

Accurate Mass: 269.040788

Percentage Composition: C 44.45%; H 6.34%; Cl 26.24%; N 5.18%; O 5.92%; S 11.87%

Melting Point: Mp 36°

>>Variant: (Z)-form

CAS Registry Number: 17708-57-5

Molecular Formula: C₁₀H₁₇Cl₂NOS

Molecular Weight: 270.222

Accurate Mass: 269.040788

Percentage Composition: C 44.45%; H 6.34%; Cl 26.24%; N 5.18%; O 5.92%; S 11.87%

Physical Description: Liq.

Refractive Index: n_D⁴⁰ 1.5124

Other Data: The more active isomer

References:

U.K. Pat., 1961, 882 111; CA, **57**, 14948b, (synth)

Verneti, J.B. et al., CA, 1966, **55**, 12795h, (use)

Rummens, F.H.A. et al., J. Agric. Food Chem., 1970, **18**, 1166, (pmr)

Rummens, F.H.A. et al., Weed Sci., 1975, **23**, 17; CA, **82**, 155235x, (isom)

de Lorenzo, F. et al., Cancer Res., 1978, **38**, 13; CA, **88**, 84295c, (tox)

IARC Monog., 1983, **30**, 235; Suppl. 7, 61, (rev, tox)

Pesticide Manual, 8th edn., 1987, 3990

Miles, C.J. et al., Anal. Chem., 1988, **60**, 220, (hplc)

Mair, P. et al., J. Agric. Food Chem., 1991, **39**, 1504, (metab)

Lewis, R.J., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold, 1992, DBI200