



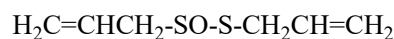
>>Entry Name: Allicin

ENTRY UNDER REVIEW

Synonym(s): S-2-Propenyl 2-propene-1-sulfinothioate, 9Cl. Allitridi

CAS Registry Number: 539-86-6

Related CAS Registry Numbers(s): 72869-75-1



Molecular Formula: C₆H₁₀OS₂

Molecular Weight: 162.276

Accurate Mass: 162.017305

Percentage Composition: C 44.41%; H 6.21%; O 9.86%; S 39.52%

Source/Synthesis: Isol. from garlic (*Allium sativum*)

Use/Importance: Shows antibacterial, antineoplastic props. and limited platelet antiaggregatory activity. Investigated for antihyperlipidaemic activity. Inhibits cholesterol synthesis *in vitro*. Antihyperglycaemic agent. Also possesses insecticidal props.

Solubility: BERDY SOL: Sol. H₂O, MeOH, Et₂O; fairly sol. hexane

UV: [neutral] λ_{max} 202 (); 240 () (MeOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, scu) 120 mg/kg. Can cause allergic contact dermatitis in sensitized rodents and individuals ; BERDY HAZD : LD₅₀ (mus, ivn) 60 mg/kg , LD₅₀ (mus, scu) 120 mg/kg

>>Variant: (±)-form

Molecular Formula: C₆H₁₀OS₂

Molecular Weight: 162.276

Accurate Mass: 162.017305

Percentage Composition: C 44.41%; H 6.21%; O 9.86%; S 39.52%

Physical Description: Yellow liq.

Density: d₂₀ 1.11

References:

- Cavallito, C.J. *et al.*, *J.A.C.S.*, 1944, **66**, 1950, (*isol, pharmacol*)
Stoll, A. *et al.*, *Helv. Chim. Acta*, 1948, **31**, 189; 1949, **32**, 197, (*synth*)
Virtanen, A.I., *Angew. Chem., Int. Ed.*, 1962, **1**, 299, (*rev*)
Isenberg, N., *Int. J. Sulfur Chem.*, 1973, **3**, 307, (*rev*)
Papageorgiou, C. *et al.*, *Arch. Dermatol. Res.*, 1983, **275**, 229, (*tox*)
Block, E. *et al.*, *J.A.C.S.*, 1986, **108**, 7045, (*synth, cmr, ir, pmr*)
Mayeux, P.R. *et al.*, *Agents Actions*, 1988, **25**, 182, (*pharmacol*)
Makheja, A.N. *et al.*, *Agents Actions*, 1990, **29**, 360, (*pharmacol*)
Gebhardt, R., *Arzneim.-Forsch.*, 1991, **41**, 800, (*pharmacol*)
Gebhardt, R. *et al.*, *Biochim. Biophys. Acta*, 1994, **1213**, 57, (*pharmacol*)
Calvey, E.M. *et al.*, *J. Chromatogr. Sci.*, 1994, **32**, 93, (*chromatog*)
Block, E. *et al.*, *Sulfur Compds. Foods*, 1993, (Eds. Mussinan, C.J. *et al.*), American Chemical Society (*ACS Symp. Ser.* v564 1994), 1994, 63, (*rev*)
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AFS250