



>>Entry Name: 1-Isothiocyanato-3-(methylthio)propane, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Methylthiopropyl isothiocyanate. **Ibervirin**. FEMA 3312

CAS Registry Number: 505-79-3

MeSCH₂CH₂CH₂NCS

Molecular Formula: C₅H₉NS₂

Molecular Weight: 147.265

Accurate Mass: 147.017639

Percentage Composition: C 40.78%; H 6.16%; N 9.51%; S 43.55%

Physical Description: Liq. with odour of radish

Boiling Point: Bp₁₂ 120.5-122°

Sigma: I1767

>>Derivative: S-Oxide

>>Derivative: S,S-Dioxide

Synonym(s): 1-Isothiocyanato-3-(methylsulfonyl)propane, 9CI. Isothiocyanopropyl methyl sulfone. 3-(Methylsulfonyl)propyl isothiocyanate. **Cheiroline**

CAS Registry Number: 505-34-0

Molecular Formula: C₅H₉NO₂S₂

Molecular Weight: 179.264

Accurate Mass: 179.007469

Percentage Composition: C 33.50%; H 5.06%; N 7.81%; O 17.85%; S 35.78%

Use/Importance: Antibacterial, antifungal agent

Physical Description: Rhombic prisms

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; fairly sol. H₂O; poorly sol. hexane

Calculated Log P Data: Log P -0.22 (calc)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ivn) 3 - 7 mg/kg

Sigma: C3182

References:

Kjaer, A. *et al.*, *Acta Chem. Scand.*, 1955, **9**, 1143; 1963, **17**, 2143, (*isol, struct, ms*)

Daxenbichler, M.E. *et al.*, *J. Agric. Food Chem.*, 1964, **12**, 127, (*occur*)

Kjaer, A. *et al.*, *Phytochemistry*, 1972, **11**, 1502; 3045,, (*isol, synth, deriv*)

Kjaer, A. *et al.*, *Chem. Scr.*, 1982, **20**, 42, (*synth*)