



>>Entry Name: 1-Propanethiol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Propyl mercaptan. 1-Mercaptopropane. FEMA 3521

CAS Registry Number: 107-03-9

Extra CAS Registry Numbers(s): 79869-58-2

$\text{H}_3\text{CCH}_2\text{CH}_2\text{SH}$

Molecular Formula: $\text{C}_3\text{H}_8\text{S}$

Molecular Weight: 76.162

Accurate Mass: 76.03467

Percentage Composition: C 47.31%; H 10.59%; S 42.10%

Source/Synthesis: Isol. from onion (*Allium cepa*)

Physical Description: Liq. Cabbage-like colour and taste

Melting Point: Mp -113.3°

Boiling Point: Bp 67°

Density: d_4^{25} 0.836

Refractive Index: n_D^{25} 1.4351

Hazard & Toxicity: Eye irritant. LD₅₀ (rat, orl) 1790 mg/kg. Highly flammable, fl. p. -20°

Aldrich: P5075-7

Fluka: 82370

>>Derivative: 3,5-Dinitrobenzoyl

Physical Description: Cryst. (AcOH aq.)

Melting Point: Mp $51-52^\circ$

>>Derivative: S-Me

Synonym(s): 1-(Methylthio)propane, 9CI. Methyl propyl sulfide, 8CI

CAS Registry Number: 3877-15-4

Molecular Formula: $\text{C}_4\text{H}_{10}\text{S}$

Molecular Weight: 90.189

Accurate Mass: 90.05032

Percentage Composition: C 53.27%; H 11.18%; S 35.55%

Physical Description: Liq.

Boiling Point: Bp 95°

>>Derivative: S-Ph

>>Derivative: S-(2,4-Dinitrophenyl)

CAS Registry Number: 7343-56-8

Melting Point: Mp $85-86^\circ$

References:

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