



>>Entry Name: 1-Hexanethiol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Hexyl mercaptan. 1-Mercaptohexane

CAS Registry Number: 111-31-9

$\text{H}_3\text{C}(\text{CH}_2)_4\text{CH}_2\text{SH}$

Molecular Formula: $\text{C}_6\text{H}_{14}\text{S}$

Molecular Weight: 118.243

Accurate Mass: 118.08162

Percentage Composition: C 60.95%; H 11.93%; S 27.12%

Physical Description: Liq.

Melting Point: Mp -81°

Boiling Point: Bp 151-152°

Density: d 0.84

Refractive Index: n_D 1.4482

Hazard & Toxicity: Flammable

Aldrich: 23419-2

Fluka: 52870

>>Derivative: S-Me

Synonym(s): 1-(Methylthio)hexane, 9CI. Hexyl methyl sulfide, 8CI

CAS Registry Number: 20291-60-5

Molecular Formula: $\text{C}_7\text{H}_{16}\text{S}$

Molecular Weight: 132.269

Accurate Mass: 132.09727

Percentage Composition: C 63.56%; H 12.19%; S 24.24%

Boiling Point: Bp₁₅ 61-62°

Rare Chemicals Library: S54015-3

Other: PB H06470

>>Derivative: S-Et

Synonym(s): 1-(Ethylthio)hexane, 9CI. Ethyl hexyl sulfide, 8CI

CAS Registry Number: 7309-44-6

Molecular Formula: $\text{C}_8\text{H}_{18}\text{S}$

Molecular Weight: 146.296

Accurate Mass: 146.11292

Percentage Composition: C 65.68%; H 12.40%; S 21.92%

Boiling Point: Bp 183-185°

Density: d 0.78

Refractive Index: n_D^{20} 1.4541

Other: PB E10780

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 256A, (ir)

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 412B, (nmr)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 336C, (ir)

Von Braun, J. *et al.*, *Annalen*, 1929, **472**, 138, (synth)

Backer, H.J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1932, **51**, 1166, (synth)

Frank, R.L. *et al.*, *J.A.C.S.*, 1946, **68**, 2103, (synth)

el Heweih, Z., *Chem. Ber.*, 1953, **86**, 862, (synth)

Parham, W.E. *et al.*, *J.O.C.*, 1962, **27**, 2698, (S-Et)

Lissel, M. *et al.*, *Synthesis*, 1986, 382, (S-Me)

Harpp, D.N. *et al.*, *Tet. Lett.*, 1986, **27**, 3975, (synth)

Gingras, M. *et al.*, *Tet. Lett.*, 1990, **31**, 1397, (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, HES000