



>>Entry Name: 3-Methyl-1-butanethiol, 9CI

Synonym(s): Isopentyl mercaptan. Isoamyl mercaptan. Isopentanethiol. Isoamyl thioalcohol. Thioisoamyl alcohol

CAS Registry Number: 541-31-1

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

Molecular Formula: $\text{C}_5\text{H}_{12}\text{S}$

Molecular Weight: 104.216

Accurate Mass: 104.06597

Percentage Composition: C 57.63%; H 11.61%; S 30.77%

Source/Synthesis: Constit. of the defence spray of the striped skunk *Mephitis mephitis*

Boiling Point: Bp 116°

Density: d_4^{20} 0.835

Refractive Index: n_D^{20} 1.4412

Hazard & Toxicity: Highly flammable, fl. p. 18°

Aldrich: 11592-4

>>Derivative: S-Me

Synonym(s): 3-Methyl-1-(methylthio)butane. Isopentyl methyl sulfide

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%

Boiling Point: Bp 136-138°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 415C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 259B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 340C, (*ir*)

Nord, F.F., *Ber.*, 1919, **52**, 1207, (*synth*)

Vejdelek, Z.J. *et al.*, *CA*, 1955, **49**, 336, (*synth*)

Obolentsev, R.D. *et al.*, *CA*, 1960, **54**, 250, (*synth*)

Andersen, K.K. *et al.*, *J. Chem. Ecol.*, 1975, **1**, 43, (*occur*)