



>>Entry Name: 1-Pentanethiol, 9CI

Synonym(s): Amyl mercaptan. 1-Mercaptopentane. *n*-Pentyl mercaptan

CAS Registry Number: 110-66-7

H3CCH2CH2CH2CH2SH

Molecular Formula: C₅H₁₂S

Molecular Weight: 104.216

Accurate Mass: 104.06597

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

Physical Description: Liq.

Boiling Point: Bp 123-124°

Density: d₂₀²⁰ 0.857

Refractive Index: n_D²⁰ 1.4437

Hazard & Toxicity: Highly flammable, fl. p. 36/18° (oc). Weak sensitiser and allergen. May cause contact dermatitis

Aldrich: P790-8

Fluka: 76960

>>Derivative: S-Ac

Synonym(s): S-Pentyl ethanethioate, 9CI

CAS Registry Number: 2432-32-8

Molecular Formula: C₇H₁₄OS

Molecular Weight: 146.253

Accurate Mass: 146.076535

Percentage Composition: C 57.49%; H 9.65%; O 10.94%; S 21.93%

Physical Description: Liq.

Boiling Point: Bp₁₄ 70-71°

>>Derivative: S-Me

Synonym(s): 1-(Methylthio)pentane, 9CI. Methyl pentyl sulfide

CAS Registry Number: 1741-83-9

Molecular Formula: C₆H₁₄S

Molecular Weight: 118.243

Accurate Mass: 118.08162

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

Physical Description: Liq.

Boiling Point: Bp 145°. Bp₂₀ 60°

Rare Chemicals Library: S35795-2

References:

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

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Wertheim, E., *J.A.C.S.*, 1929, **51**, 3661, (*synth*)

Cossar, B.C. *et al.*, *J.O.C.*, 1962, **27**, 93, (*synth*)

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