



>>Entry Name: 1-Pentanethiol, 9CI

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

CAS Registry Number: 110-66-7

H3CCH2CH2CH2CH2SH

Molecular Formula: C<sub>5</sub>H<sub>12</sub>S

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: d<sub>20</sub><sup>20</sup> 0.857

Refractive Index: n<sub>D</sub><sup>20</sup> 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: C<sub>7</sub>H<sub>14</sub>OS

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: Bp<sub>14</sub> 70-71°

>>Derivative: S-Me

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

CAS Registry Number: 1741-83-9

Molecular Formula: C<sub>6</sub>H<sub>14</sub>S

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°. Bp<sub>20</sub> 60°

Rare Chemicals Library: S35795-2

#### References:

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

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 255D, (ir)

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*Aldrich Library of FT-NMR Spectra*, **1**, 412A, (nmr)

*Sadtler Standard C-13 NMR Spectra*, 12295, (cmr)

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

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

Savignac, P. *et al.*, *Synthesis*, 1974, 818, (derivs)

Černý, M. *et al.*, *Coll. Czech. Chem. Comm.*, 1983, **48**, 1749, (ms)

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