



>>Entry Name: 1-Octanethiol, 9CI

Synonym(s): Octyl mercaptan. 1-Mercaptooctane

CAS Registry Number: 111-88-6

$\text{H}_3\text{C}(\text{CH}_2)_6\text{CH}_2\text{SH}$

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%

Physical Description: Liq. with powerful unpleasant odour

Boiling Point: Bp 197-200°. Bp₁₀ 77-78°

Hazard & Toxicity: Fl. p. 69° (oc)

Aldrich: 13124-5

Fluka: 74890

>>Derivative: S-Ac

Molecular Formula: $\text{C}_{10}\text{H}_{20}\text{OS}$

Molecular Weight: 188.333

Accurate Mass: 188.123485

Percentage Composition: C 63.78%; H 10.70%; O 8.50%; S 17.03%

Physical Description: Liq.

Boiling Point: Bp₁₀ 116-117°

>>Derivative: S-Me

Synonym(s): 1-(Methylthio)octane, 9CI. Methyl octyl sulfide

CAS Registry Number: 3698-95-1

Molecular Formula: $\text{C}_9\text{H}_{20}\text{S}$

Molecular Weight: 160.323

Accurate Mass: 160.12857

Percentage Composition: C 67.43%; H 12.57%; S 20.00%

Boiling Point: Bp₂₀ 104-105°

Other: PB M23950

>>Derivative: S-Et

Synonym(s): 1-(Ethylthio)octane. Ethyl 1-octyl sulfide

CAS Registry Number: 3698-94-0

Molecular Formula: $\text{C}_{10}\text{H}_{22}\text{S}$

Molecular Weight: 174.35

Accurate Mass: 174.14422

Percentage Composition: C 68.89%; H 12.72%; S 18.39%

Boiling Point: Bp₁₄ 108-110°

Rare Chemicals Library: S57065-6

References:

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Bateman, L. *et al.*, *J.C.S.*, 1958, 2838, (*synth, bibl*)

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Mori, K. *et al.*, *J.O.C.*, 1969, **34**, 4170, (*synth*)

Degani, I. *et al.*, *Synthesis*, 1977, 873; 1979, 178, (*synth, S-Me*)

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