



>>Entry Name: 1-Hexadecanethiol, 9CI

Synonym(s): Cetyl mercaptan. 1-Mercaptohexadecane

CAS Registry Number: 2917-26-2

$\text{H}_3\text{C}(\text{CH}_2)_{14}\text{CH}_2\text{SH}$

Molecular Formula: $\text{C}_{16}\text{H}_{34}\text{S}$

Molecular Weight: 258.511

Accurate Mass: 258.23812

Percentage Composition: C 74.34%; H 13.26%; S 12.40%

Boiling Point: Bp_2 170-179°. $\text{Bp}_{0.5}$ 123-128°

Aldrich: H763-7

Fluka: 52270

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 414B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 257B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 338C, (*ir*)

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

Baer, J.E. *et al.*, *J.A.C.S.*, 1949, **71**, 1215, (*uv*)

Farlow, M.W. *et al.*, *Ind. Eng. Chem.*, 1950, **42**, 2547, (*synth*)

O'Donnell, D.C. *et al.*, *J.A.C.S.*, 1955, **77**, 3154