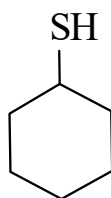




>>Entry Name: Cyclohexanethiol, 9CI

Synonym(s): Hexahydrothiophenol. Mercaptocyclohexane. Cyclohexyl mercaptan



CAS Registry Number: 1569-69-3

Molecular Formula: C₆H₁₂S

Molecular Weight: 116.227

Accurate Mass: 116.06597

Percentage Composition: C 62.00%; H 10.41%; S 27.59%

Physical Description: Oil

Boiling Point: Bp 158-160° (155°)

Solubility: Sol. EtOH, CHCl₃, insol. H₂O

Density: d⁰ 0.991

Refractive Index: n_D²⁰ 1.4911

Other Data: Steam-volatile

Hazard & Toxicity: Eye and skin irritant. Flammable, fl. p. 43°

Aldrich: C10560-0

Fluka: 29461

>>Derivative: Ac

Synonym(s): S-Cyclohexyl ethanethioate

CAS Registry Number: 10039-63-1

Molecular Formula: C₈H₁₄OS

Molecular Weight: 158.264

Accurate Mass: 158.076535

Percentage Composition: C 60.71%; H 8.92%; O 10.11%; S 20.26%

Boiling Point: Bp₁₅ 90-91°

>>Derivative: Benzoyl

Synonym(s): S-Cyclohexyl benzenecarbothioate

CAS Registry Number: 10035-90-2

Molecular Formula: C₁₃H₁₆OS

Molecular Weight: 220.335

Accurate Mass: 220.092185

Percentage Composition: C 70.87%; H 7.32%; O 7.26%; S 14.55%

Boiling Point: Bp₂ 123-125°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 418A, (*nmr*)

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

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 341C, (*ir*)

Borsche, W. *et al.*, *Ber.*, 1906, **39**, 393, (*synth*)

Schneider, H.J., *J.O.C.*, 1978, **43**, 3866, (*cmr*)

Lucien, J. *et al.*, *Nouv. J. Chim.*, 1979, **3**, 15, (*synth*)

Wilson, S.R. *et al.*, *J.A.C.S.*, 1980, **102**, 3577, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, CPB625