



>>Entry Name: **3-Hexanethiol**, 9CI

Synonym(s): 3-Mercaptohexane

CAS Registry Number: 1633-90-5

H3CCH2CH2CH(SH)CH2CH3

Molecular Formula: C₆H₁₄S

Molecular Weight: 118.243

Accurate Mass: 118.08162

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

>>Variant: (±)-form

CAS Registry Number: 110503-15-6

Molecular Formula: C₆H₁₄S

Molecular Weight: 118.243

Accurate Mass: 118.08162

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

Boiling Point: Bp₁₃ 30.5-31°. Bp₂₅ 57°

Density: d₂₀²⁰ 0.832

Refractive Index: n_D²⁰ 1.4428

References:

Spiegler, L. *et al.*, *J.A.C.S.*, 1939, **61**, 940, (*synth*)

Akerstrom, S., *Ark. Kemi*, 1965, **24**, 505; *CA*, **63**, 17880f, (*synth*)