



>>Entry Name: 2-(Phenylthio)ethanol, 9CI

Synonym(s): 2-Phenylmercaptoethanol. 2-Hydroxyethyl phenyl sulfide

CAS Registry Number: 699-12-7

PhSCH₂CH₂OH

Molecular Formula: C₈H₁₀OS

Molecular Weight: 154.232

Accurate Mass: 154.045235

Percentage Composition: C 62.30%; H 6.53%; O 10.37%; S 20.79%

Use/Importance: Useful protecting agent group in oligonucleotide synth.

Physical Description: Liq. with sweet odour

Boiling Point: Bp₈ 135°

Density: d₁₅²⁴ 1.115

Refractive Index: n_D²⁰ 1.5876

Aldrich: 23277-7

Fluka: 54420

Sigma: P2778

>>Derivative: S,S-Dioxide

Synonym(s): 2-(Phenylsulfonyl)ethanol

CAS Registry Number: 20611-21-6

Molecular Formula: C₈H₁₀O₃S

Molecular Weight: 186.231

Accurate Mass: 186.035065

Percentage Composition: C 51.60%; H 5.41%; O 25.77%; S 17.22%

Melting Point: Mp 18-20°

Boiling Point: Bp₂ 177°. Bp_{0.15} 131°

Refractive Index: n_D²⁴ 1.5555

Aldrich: 36068-6

>>Derivative: Ac

CAS Registry Number: 20965-30-4

Molecular Formula: C₁₀H₁₂O₂S

Molecular Weight: 196.27

Accurate Mass: 196.0558

Percentage Composition: C 61.20%; H 6.16%; O 16.30%; S 16.34%

Physical Description: Liq.

Boiling Point: Bp₁ 111-112°

Rare Chemicals Library: S86639-3

>>Derivative: 4-Nitrobenzoyl

Physical Description: Cryst. (MeOH)

Melting Point: Mp 57-58°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1176B, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 434B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1092D, (*ir*)

Kirner, W.R. *et al.*, *J.A.C.S.*, 1929, **51**, 3409-3418, (*synth*)

Schultz, H.S. *et al.*, *J.O.C.*, 1963, **28**, 1140-1142, (*synth, dioxide*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 516, (*use*)

Tamura, Y. *et al.*, *Synthesis*, 1975, 641-642, (*synth*)

Julia, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1976, 519-524, (*synth, dioxide*)

Bangov, I.P. *et al.*, *Org. Magn. Reson.*, 1983, **21**, 443-449, (*cmr*)