



>>Entry Name: 4-Mercaptobenzenemethanol

Synonym(s): 4-Mercaptobenzyl alcohol. 4-(Hydroxymethyl)thiophenol

CAS Registry Number: 53339-53-0

Molecular Formula: C₇H₈OS

Molecular Weight: 140.206

Accurate Mass: 140.029585

Percentage Composition: C 59.97%; H 5.75%; O 11.41%; S 22.87%

Physical Description: Plates (CCl₄/petrol)

Melting Point: Mp 52-54°

>>Derivative: S-Me

CAS Registry Number: 3446-90-0

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%

Physical Description: Cryst.

Melting Point: Mp 37-39°

Boiling Point: Bp_{0.01} 100°

Aldrich: 23068-5

>>Derivative: Disulfide

Molecular Formula: C₁₄H₁₄O₂S₂

Molecular Weight: 278.395

Accurate Mass: 278.04352

Percentage Composition: C 60.40%; H 5.07%; O 11.49%; S 23.04%

Physical Description: Needles (Me₂CO aq.)

Melting Point: Mp 130-132°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 438B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1186A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1106A, (*ir*)

Grice, R. *et al.*, *J.C.S.*, 1963, 1947, (*synth*)

Itoh, T. *et al.*, *J.O.C.*, 1996, **61**, 1867, (*synth, ir, pmr, cmr, ms*)