



>>Entry Name: Benzyl phenyl sulfide, 8Cl

Synonym(s): [(Phenylmethyl)thio]benzene, 9Cl

CAS Registry Number: 831-91-4

PhSCH₂Ph

Molecular Formula: C₁₃H₁₂S

Molecular Weight: 200.304

Accurate Mass: 200.06597

Percentage Composition: C 77.95%; H 6.04%; S 16.01%

Melting Point: Mp 43-44°

Boiling Point: Bp₂₇ 197°. Bp₁₄ 145-155°

Aldrich: B2920-2

Fluka: 13775

>>Derivative: S-Oxide

see Benzyl phenyl sulfoxide, [CXT26-B](#)

>>Derivative: S,S-Dioxide

Synonym(s): [(Phenylmethyl)sulfonyl]benzene, 9Cl. Benzyl phenyl sulfone

CAS Registry Number: 3112-88-7

Molecular Formula: C₁₃H₁₂O₂S

Molecular Weight: 232.303

Accurate Mass: 232.0558

Percentage Composition: C 67.22%; H 5.21%; O 13.77%; S 13.80%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 149-150.5°

Hazard & Toxicity: LD₅₀ (mus, ivn) 320 mg/kg

Rare Chemicals Library: S61443-2

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1184B, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 444B, (*nmr*)

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Sadtler Standard C-13 NMR Spectra, (*cmr*)

Sadtler Standard NMR Spectra, 23285, (*pmr*)

Sadtler Standard Ultraviolet Spectra, 8477, (*uv*)

Bordwell, F.G. *et al.*, *J.A.C.S.*, 1955, **77**, 572, (*synth*)

Bowie, J.H. *et al.*, *J.C.S.(B)*, 1966, 951, (*ms*)

Wladislaw, B. *et al.*, *J.C.S.(B)*, 1971, 2037, (*ir*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 131, (*use*)

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