



>>Entry Name: Chloromethyl phenyl sulfide, 8Cl

Synonym(s): [(Chloromethyl)thio]benzene, 9Cl. Phenylthiomethyl chloride

CAS Registry Number: 7205-91-6

PhSCH₂Cl

Molecular Formula: C₇H₇ClS

Molecular Weight: 158.651

Accurate Mass: 157.995697

Percentage Composition: C 52.99%; H 4.45%; Cl 22.35%; S 20.21%

Boiling Point: Bp₁₂ 104°. Bp_{1.5} 83°

Aldrich: 21663-1

Fluka: 25201

>>Derivative: S-Oxide

Synonym(s): [(Chloromethyl)sulfinyl]benzene. Chloromethyl phenyl sulfoxide

CAS Registry Number: 7205-94-9

Molecular Formula: C₇H₇ClOS

Molecular Weight: 174.65

Accurate Mass: 173.990612

Percentage Composition: C 48.14%; H 4.04%; Cl 20.30%; O 9.16%; S 18.36%

Use/Importance: Reagent for synth. of chloromethyl ketones and α,β-unsatd. aldehydes

Melting Point: Mp 38.5-39.5°

Boiling Point: Bp₁ 120-122°

Fluka: 25205

>>Derivative: S,S-Dioxide

Synonym(s): [(Chloromethyl)sulfonyl]benzene. Chloromethyl phenyl sulfone

CAS Registry Number: 7205-98-3

Molecular Formula: C₇H₇ClO₂S

Molecular Weight: 190.65

Accurate Mass: 189.985527

Percentage Composition: C 44.10%; H 3.70%; Cl 18.60%; O 16.78%; S 16.82%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 52-53° (47-49°)

Aldrich: 32460-4

Fluka: 25202

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 1182B, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 433B; 1581B, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1100C, (*ir*)
Hsieh, H.-H. *et al.*, *J.O.C.*, 1973, **38**, 17, (*synth*)
Bordwell, F.G. *et al.*, *J.O.C.*, 1974, **39**, 2516, (*sulfone*)
Hojo, M. *et al.*, *Synthesis*, 1976, 697, (*synth*)
Hanske, J.R. *et al.*, *J.O.C.*, 1979, **44**, 2472, (*synth*)
Davis, P.P. *et al.*, *Org. Mass Spectrom.*, 1979, **12**, 659, (*synth, ms*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 94; 1984, **12**, 439
Ono, N. *et al.*, *Synthesis*, 1980, 952, (*synth*)
Campbell, M.M. *et al.*, *Tet. Lett.*, 1980, 3305, (*synth*)
O'Connor, E.J. *et al.*, *J.A.C.S.*, 1987, **109**, 3739, (*synth, pmr*)
Katritzky, A.R. *et al.*, *J.C.S. Perkin 1*, 1987, 769, (*synth*)
Cadman, M.L.F. *et al.*, *J.C.S. Perkin 1*, 1995, 1397, (*oxide, synth, pmr*)
Silveira, C.C. *et al.*, *Synth. Commun.*, 1995, **25**, 117, (*synth, pmr, ms*)
Org. Synth., 2000, **78**, 169-176, (*synth, ir, pmr, cmr*)