



>>Entry Name: Fluoromethyl phenyl sulfide

Synonym(s): [(Fluoromethyl)thio]benzene, 9CI. Phenyl fluoromethyl sulfide

CAS Registry Number: 60839-94-3

PhSCH₂F

Molecular Formula: C₇H₇FS

Molecular Weight: 142.197

Accurate Mass: 142.025248

Percentage Composition: C 59.13%; H 4.96%; F 13.36%; S 22.55%

Physical Description: Liq.

Boiling Point: Bp_{0.1} 80-90°

Refractive Index: n_D²² 1.5503

Other Data: Polymerises rapidly. Dec. on heating

>>Derivative: S-Oxide, (±)-form

Synonym(s): Fluoromethyl phenyl sulfoxide

CAS Registry Number: 65325-68-0

Molecular Formula: C₇H₇FOS

Molecular Weight: 158.196

Accurate Mass: 158.020163

Percentage Composition: C 53.15%; H 4.46%; F 12.01%; O 10.11%; S 20.27%

Physical Description: Liq.

Refractive Index: n_D²² 1.5575

>>Derivative: S,S-Dioxide

Synonym(s): Fluoromethyl phenyl sulfone, 8CI

CAS Registry Number: 20808-12-2

Molecular Formula: C₇H₇FO₂S

Molecular Weight: 174.195

Accurate Mass: 174.015078

Percentage Composition: C 48.27%; H 4.05%; F 10.91%; O 18.37%; S 18.41%

Use/Importance: Fluoromethyl Wittig equivalent

Physical Description: Cryst. (hexane)

Melting Point: Mp 52-53° (47-48°)

References:

Yagupolskii, L.M. *et al.*, *Zh. Obshch. Khim.*, 1968, **38**, 1503-1509; *CA*, **70**, 3436c, (*dioxide, synth*)

Zupan, M., *J. Fluorine Chem.*, 1976, **8**, 305-309, (*synth, ms, pmr*)

More, K.M. *et al.*, *Synthesis*, 1977, 791-792, (*oxide, synth, pmr*)

Inbasekaran, M. *et al.*, *Chem. Comm.*, 1985, 678-679, (*synth, use, dioxide*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1988, **13**, 135-136, (*use, dioxide*)

Fuchigami, T. *et al.*, *J.O.C.*, 1994, **59**, 5937-5941, (*dioxide, synth, pmr, F-19 nmr, ir*)

Matthews, D.P. *et al.*, *Org. Prep. Proced. Int.*, 1994, **26**, 605-608, (*synth, dioxide*)

Org. Synth., Coll. Vol., 9, 1998, 446-449, (*dioxide, synth pmr, F-19 nmr*)