



>>Entry Name: Difluoromethyl phenyl sulfide, 8Cl

Synonym(s): [(Difluoromethyl)thio]benzene, 9Cl. Phenyl difluoromethyl sulfide

CAS Registry Number: 1535-67-7

PhSCHF₂

Molecular Formula: C₇H₆F₂S

Molecular Weight: 160.187

Accurate Mass: 160.015826

Percentage Composition: C 52.49%; H 3.78%; F 23.72%; S 20.02%

Physical Description: Liq.

Boiling Point: Bp₇ 62-63°

Density: d₄²⁵ 1.222

Refractive Index: n_D²⁵ 1.5084

Other Data: Part. dec.>ca. 60°

>>Derivative: S-Oxide

Synonym(s): Difluoromethyl phenyl sulfoxide, 8Cl

CAS Registry Number: 24933-64-0

Molecular Formula: C₇H₆F₂OS

Molecular Weight: 176.187

Accurate Mass: 176.010741

Percentage Composition: C 47.72%; H 3.43%; F 21.57%; O 9.08%; S 18.20%

Physical Description: Liq.

Boiling Point: Bp₁₀ 121-122°

Density: d₂₃ 1.328

Refractive Index: n_D²³ 1.5266

>>Derivative: S,S-Dioxide

Synonym(s): Difluoromethyl phenyl sulfone, 8Cl

CAS Registry Number: 1535-65-5

Molecular Formula: C₇H₆F₂O₂S

Molecular Weight: 192.186

Accurate Mass: 192.005656

Percentage Composition: C 43.75%; H 3.15%; F 19.77%; O 16.65%; S 16.68%

Physical Description: Liq.

Melting Point: Mp 24.7-25°

Boiling Point: Bp₇ 115-120°

Density: d₄²⁷ 1.324

Refractive Index: n_D²⁷ 1.4999

References:

Hine, J. *et al.*, *J.A.C.S.*, 1957, **79**, 5493; 1960, **82**, 6178, (*synth, sulfone*)

Sedova, L.N. *et al.*, *Zh. Obshch. Khim.*, 1969, **39**, 2057; *CA*, **72**, 31366q, (*sulfoxide*)

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