



>>Entry Name: Phenyl trifluoromethyl sulfide

Synonym(s): [(Trifluoromethyl)thio]benzene, 9CI

CAS Registry Number: 456-56-4

PhSCF₃

Molecular Formula: C₇H₅F₃S

Molecular Weight: 178.178

Accurate Mass: 178.006404

Percentage Composition: C 47.19%; H 2.83%; F 31.99%; S 18.00%

Boiling Point: Bp 140-142°

>>Derivative: S-Oxide

Synonym(s): Phenyl trifluoromethyl sulfoxide. [(Trifluoromethyl)sulfinyl]benzene

CAS Registry Number: 703-18-4

Molecular Formula: C₇H₅F₃OS

Molecular Weight: 194.177

Accurate Mass: 194.001319

Percentage Composition: C 43.30%; H 2.60%; F 29.35%; O 8.24%; S 16.51%

Boiling Point: Bp₁₀ 82-83°

Refractive Index: n_D²⁰ 1.4728

>>Derivative: S,S-Dioxide

Synonym(s): Phenyl trifluoromethyl sulfone. [(Trifluoromethyl)sulfonyl]benzene

CAS Registry Number: 426-58-4

Molecular Formula: C₇H₅F₃O₂S

Molecular Weight: 210.176

Accurate Mass: 209.996234

Percentage Composition: C 40.00%; H 2.40%; F 27.12%; O 15.22%; S 15.26%

Boiling Point: Bp₃₀ 110°

References:

Schuster, I.I.M., *J. Magn. Reson.*, 1975, **17**, 104, (*cmr*, *F-19 nmr*)

Hendrickson, J.B. *et al.*, *J.O.C.*, 1977, **42**, 3875, (*dioxide*)

Popov, V.I. *et al.*, *J. Fluorine Chem.*, 1982, **21**, 365, (*synth*)

Kondratenko, N. *et al.*, *Zh. Org. Khim.*, 1989, **25**, 1116; *J. Org. Chem. USSR (Engl. Transl.)*, 1989, **25**, 1005, (*oxide*)

Clark, J.H. *et al.*, *J. Fluorine Chem.*, 1990, **48**, 249, (*synth*)

Yang, J.-J. *et al.*, *J.O.C.*, 1998, **63**, 2656-2660, (*oxide*, *dioxide*, *synth*, *ir*, *pmr*, *cmr*, *ms*)