



>>Entry Name: 2,3,5,6-Tetrafluorobenzenethiol, 9Cl, 8Cl

ENTRY UNDER REVIEW

Synonym(s): 2,3,5,6-Tetrafluorothiophenol. 1,2,4,5-Tetrafluoro-3-mercaptobenzene

CAS Registry Number: 769-40-4

Molecular Formula: C₆H₂F₄S

Molecular Weight: 182.141

Accurate Mass: 181.981332

Percentage Composition: C 39.57%; H 1.11%; F 41.72%; S 17.61%

Physical Description: Liq.

Boiling Point: Bp 152-153°

Refractive Index: n_D²² 1.4827

Aldrich: 10018-8

>>Derivative: S-Me

Synonym(s): 1,2,4,5-Tetrafluoro-3-(methylthio)benzene, 9Cl. Methyl 2,3,5,6-tetrafluorophenyl sulfide. 1,2,4,5-Tetrafluorophenyl methyl sulfide

CAS Registry Number: 1480-02-0

Molecular Formula: C₇H₄F₄S

Molecular Weight: 196.168

Accurate Mass: 195.996982

Percentage Composition: C 42.86%; H 2.06%; F 38.74%; S 16.35%

Physical Description: Liq.

Boiling Point: Bp 169-174°

>>Derivative: S-Et

Synonym(s): 3-(Ethylthio)-1,2,4,5-tetrafluoroethylbenzene, 9Cl. Ethyl 2,3,5,6-tetrafluorophenyl sulfide

CAS Registry Number: 78522-94-8

Molecular Formula: C₈H₆F₄S

Molecular Weight: 210.195

Accurate Mass: 210.012632

Percentage Composition: C 45.71%; H 2.88%; F 36.15%; S 15.26%

Boiling Point: Bp₁₁ 87-88°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 429B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1181A, (*ir*)

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Aldrich Library of NMR Spectra, 2nd Ed., **2**, 982A, (*pmr*)

Sigma-Aldrich Library of Chemical Safety Data, 1st Ed., 1665D, (*haz*)

Robson, P. *et al.*, *J.C.S.*, 1960, 4754, (*synth*, *uv*, *ir*)

Netherlands Pat., 1966, 6 605 036; *CA*, **66**, 65492u, (*synth*)

Wasylishen, R. *et al.*, *Can. J. Chem.*, 1970, **48**, 2885, (*pmr*)