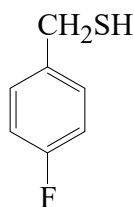




>>Entry Name: 4-Fluorobenzenemethanethiol, 9CI

Synonym(s): *p*-Fluoro- α -toluenethiol, 8CI. 4-Fluorobenzyl mercaptan



CAS Registry Number: 15894-04-9

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%

Boiling Point: Bp₆ 69°

>>Derivative: *S*-Me

Synonym(s): 1-Fluoro-4-[(methylthio)methyl]benzene, 9CI. 4-Fluorobenzyl methyl sulfide

CAS Registry Number: 5925-85-9

Molecular Formula: C₈H₉FS

Molecular Weight: 156.224

Accurate Mass: 156.040898

Percentage Composition: C 61.51%; H 5.81%; F 12.16%; S 20.53%

Physical Description: Oil

Boiling Point: Bp₁₈ 98°. Bp_{1.5} 60-61.5°

>>Derivative: *S*-Me, *S,S*-dioxide

Synonym(s): 1-Fluoro-4-[(methylsulfonyl)methyl]benzene, 9CI. 4-Fluorobenzyl methyl sulfone

CAS Registry Number: 5925-83-7

Molecular Formula: C₈H₉FO₂S

Molecular Weight: 188.222

Accurate Mass: 188.030728

Percentage Composition: C 51.05%; H 4.82%; F 10.09%; O 17.00%; S 17.04%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 105°

>>Derivative: *S*-Ph

Synonym(s): 1-Fluoro-4-[(phenylthio)methyl]benzene, 9CI. 4-Fluorobenzyl phenyl sulfide

CAS Registry Number: 351-66-6

Molecular Formula: C₁₃H₁₁FS

Molecular Weight: 218.294

Accurate Mass: 218.056548

Percentage Composition: C 71.53%; H 5.08%; F 8.70%; S 14.69%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 62-62.5°

References:

U.K. Pat., 1956, 748 604; CA, **51**, 1267h, (*S*-Ph)

Mayer, R. *et al.*, Chem. Ber., 1966, **99**, 1393, (*S*-Me)

Paquette, L.A. *et al.*, J.O.C., 1968, **33**, 1080, (*synth*)

Adcock, W. *et al.*, J.A.C.S., 1973, **95**, 7353, (*synth*, *F-19 nmr*)

Schaefer, T. *et al.*, J. Magn. Reson., 1980, **41**, 395, (*pmr*)