



>>Entry Name: 4-Fluorobenzenethiol, 9CI

Synonym(s): 1-Fluoro-4-mercaptobenzene. 4-Fluorothiophenol

CAS Registry Number: 371-42-6

Structure by analogy with 2-Fluorobenzenethiol, [GZK35-Q](#)

Molecular Formula: C₆H₅FS

Molecular Weight: 128.17

Accurate Mass: 128.009598

Percentage Composition: C 56.23%; H 3.93%; F 14.82%; S 25.02%

Boiling Point: Bp 162°. Bp_{2,3} 29-30°

Refractive Index: n_D²⁵ 1.5485

Aldrich: F1531-5

Fluka: 47510

>>Derivative: S-Me

Synonym(s): 1-Fluoro-4-(methylthio)benzene. *p*-Fluorophenyl methyl sulfide, 8CI. 4-Fluorothioanisole

CAS Registry Number: 371-15-3

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: Bp 184-185°. Bp₃₁ 89-90°

Aldrich: 46769-3

Other: Oakwood 3730

>>Derivative: S-Me, S-oxide (±)

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%

Boiling Point: Bp₃ 114-115°

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

CAS Registry Number: 455-15-2

Molecular Formula: C₇H₇FO₂S

Molecular Weight: 174.196

Accurate Mass: 174.015078

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

Melting Point: Mp 78-81°

Aldrich: 18433-0

>>Derivative: S-Trifluoromethyl

Synonym(s): 1-Fluoro-4-(trifluoromethylthio)benzene. *p*-Fluorophenyl trifluoromethyl sulfide

CAS Registry Number: 940-76-1

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%

Boiling Point: Bp 138°

Density: d₂₀¹⁸ 1.355

>>Derivative: S-Trifluoromethyl, S,S-dioxide

Synonym(s): 1-Fluoro-4-(trifluoromethylsulfonyl)benzene. *p*-Fluorophenyl trifluoromethyl sulfone

CAS Registry Number: 944-30-9

Molecular Formula: C₇H₄F₄O₂S

Molecular Weight: 228.167

Accurate Mass: 227.986812

Percentage Composition: C 36.85%; H 1.77%; F 33.31%; O 14.02%; S 14.05%

Boiling Point: Bp 196-197°

Sigma: C7529

>>Derivative: Disulfide