



>>Entry Name: 3-Fluorobenzenesulfonic acid

CAS Registry Number: 657-47-6

Structure by analogy with 2-Fluorobenzenesulfonic acid, [FFW67-O](#)

Molecular Formula: C₆H₅FO₃S

Molecular Weight: 176.168

Accurate Mass: 175.994343

Percentage Composition: C 40.91%; H 2.86%; F 10.78%; O 27.25%; S 18.20%

Boiling Point: Bp 84.8°

Refractive Index: n_D³⁰ 1.4610

>>Derivative: Et ester

Molecular Formula: C₈H₉FO₃S

Molecular Weight: 204.222

Accurate Mass: 204.025643

Percentage Composition: C 47.05%; H 4.44%; F 9.30%; O 23.50%; S 15.70%

Boiling Point: Bp₂ 90-91°

>>Derivative: Fluoride

Molecular Formula: C₆H₄F₂O₂S

Molecular Weight: 178.159

Accurate Mass: 177.990006

Percentage Composition: C 40.45%; H 2.26%; F 21.33%; O 17.96%; S 18.00%

Boiling Point: Bp₂₀ 78-82°

>>Derivative: Chloride

CAS Registry Number: 701-27-9

Molecular Formula: C₆H₄ClFO₂S

Molecular Weight: 194.614

Accurate Mass: 193.960455

Percentage Composition: C 37.03%; H 2.07%; Cl 18.22%; F 9.76%; O 16.44%; S 16.48%

Melting Point: Mp 7°

Boiling Point: Bp₁₃ 109-110°

Refractive Index: n_D²⁰ 1.5308

Other: Oakwood 3575

>>Derivative: Amide

Molecular Formula: C₆H₆FNO₂S

Molecular Weight: 175.183

Accurate Mass: 175.010327

Percentage Composition: C 41.14%; H 3.45%; F 10.84%; N 8.00%; O 18.27%; S 18.30%

Melting Point: Mp 128.5-129.5°

>>Derivative: Anilide

Molecular Formula: C₁₂H₁₀FNO₂S

Molecular Weight: 251.281

Accurate Mass: 251.041627

Percentage Composition: C 57.36%; H 4.01%; F 7.56%; N 5.57%; O 12.73%; S 12.76%

Melting Point: Mp 75-76°

References:

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Prinsen, A.J. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1965, **84**, 24, (*derivs*)

Karavaev, B.I. *et al.*, *CA*, 1972, **76**, 30438k, (*uv*)

Suzuki, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 2010, (*fluoride*)