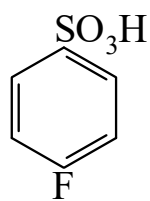




>>Entry Name: 4-Fluorobenzenesulfonic acid



CAS Registry Number: 368-88-7

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%

Use/Importance: Anthelmintic for domestic animals. Also has insecticidal properties.

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 87°

>>Derivative: Chloride

CAS Registry Number: 349-88-2

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 35°

Boiling Point: Bp_{2.2} 95-96°

Aldrich: F620-6

Fluka: 46670

Sigma: F9250

>>Derivative: Amide

CAS Registry Number: 402-46-0

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%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 126°

Hazard & Toxicity: LD₅₀ (mus, ipr) 562 mg/kg

Rare Chemicals Library: S44212-7

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1621A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 520C, (*ir*)

Oláh, P., *Acta Chim. Acad. Sci. Hung.*, 1954, **4**, 111

Taft, R.W. *et al.*, *J.A.C.S.*, 1963, **85**, 3146, (*nmr*)

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