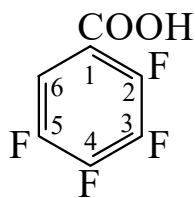




>>Entry Name: 2,3,4,5-Tetrafluorobenzoic acid



CAS Registry Number: 1201-31-6

Molecular Formula: C₇H₂F₄O₂

Molecular Weight: 194.085

Accurate Mass: 193.999092

Percentage Composition: C 43.32%; H 1.04%; F 39.15%; O 16.49%

Physical Description: Cryst. (petrol)

Melting Point: Mp 85.5-87°

Aldrich: 32626-7

Fluka: 87260

>>Derivative: Me ester

CAS Registry Number: 5292-42-2

Molecular Formula: C₈H₄F₄O₂

Molecular Weight: 208.112

Accurate Mass: 208.014742

Percentage Composition: C 46.17%; H 1.94%; F 36.52%; O 15.38%

Physical Description: Liq.

Boiling Point: Bp 187-188°

>>Derivative: Chloride

CAS Registry Number: 94695-48-4

Molecular Formula: C₇HCIF₄O

Molecular Weight: 212.531

Accurate Mass: 211.965204

Percentage Composition: C 39.56%; H 0.47%; Cl 16.68%; F 35.76%; O 7.53%

Physical Description: Yellowish oil

>>Derivative: Nitrile

Synonym(s): 2,3,4,5-Tetrafluorobenzonitrile. 1-Cyano-2,3,4,5-tetrafluorobenzene

CAS Registry Number: 16582-93-7

Molecular Formula: C₇HF₄N

Molecular Weight: 175.085

Accurate Mass: 175.004511

Percentage Composition: C 48.02%; H 0.58%; F 43.40%; N 8.00%

Physical Description: Liq.

Boiling Point: Bp 164-165°

Aldrich: 33719-6

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1155B; 1541C, (*nmr*)

Yakobson, G.G. *et al.*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1966, **36**, 144, (*synth, deriv*)

Belf, L.J. *et al.*, *Tetrahedron*, 1967, **23**, 4719, (*synth, deriv*)

Tamborski, C. *et al.*, *J. Organomet. Chem.*, 1969, **17**, 185, (*synth*)