



>>Entry Name: 2,3,5,6-Tetrafluorobenzoic acid

CAS Registry Number: 652-18-6

Molecular Formula: $C_7H_2F_4O_2$

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. (toluene)

Melting Point: Mp 154°

Aldrich: 30362-3

Sigma: T5652

>>Derivative: Nitrile

Synonym(s): 2,3,5,6-Tetrafluorobenzonitrile. 3-Cyano-1,2,4,5-tetrafluorobenzene

CAS Registry Number: 5216-17-1

Molecular Formula: C_7HF_4N

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: Bp₄₅ 88-90°

Aldrich: 30317-8

Sigma: T5777

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1155C; 1542A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1420C, (*ir*)

Alsop, D.J. *et al.*, *J.C.S.*, 1962, 1801, (*synth*)

Vysochin, N.N. *et al.*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1969, **39**, 1607, (*synth*)