



>>Entry Name: 2,4-Difluorobenzoic acid

CAS Registry Number: 1583-58-0

Molecular Formula: $C_7H_4F_2O_2$

Molecular Weight: 158.104

Accurate Mass: 158.017936

Percentage Composition: C 53.18%; H 2.55%; F 24.03%; O 20.24%

Physical Description: Cryst.

Melting Point: Mp 185°

Aldrich: 26429-6

>>Derivative: Et ester

Molecular Formula: $C_9H_8F_2O_2$

Molecular Weight: 186.158

Accurate Mass: 186.049236

Percentage Composition: C 58.07%; H 4.33%; F 20.41%; O 17.19%

Boiling Point: Bp₁₅ 65-67°

>>Derivative: Chloride

CAS Registry Number: 72482-64-5

Molecular Formula: $C_7H_3ClF_2O$

Molecular Weight: 176.55

Accurate Mass: 175.984048

Percentage Composition: C 47.62%; H 1.71%; Cl 20.08%; F 21.52%; O 9.06%

Physical Description: Liq.

Boiling Point: Bp₁₉ 68-70°

Aldrich: 26529-2

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2,4-difluorobenzene

CAS Registry Number: 3939-09-1

Molecular Formula: $C_7H_3F_2N$

Molecular Weight: 139.104

Accurate Mass: 139.023355

Percentage Composition: C 60.44%; H 2.17%; F 27.32%; N 10.07%

Physical Description: Cryst.

Melting Point: Mp 47-49°

Aldrich: 26432-6

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **2**, 1104B; 1347A; 1530B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1330B; 1417C, (*ir*)

Lock, G., *Monatsh. Chem.*, 1959, **90**, 680, (*synth*)

Hopf, H. *et al.*, *J.O.C.*, 1962, **27**, 2923, (*synth*)

Finger, G.C. *et al.*, *Chem. Comm.*, 1965, 430, (*deriv*)

Anderson, W. *et al.*, *J. Med. Chem.*, 1982, **25**, 84, (*synth, deriv*)