



>>Entry Name: 3,5-Difluorobenzoic acid

CAS Registry Number: 455-40-3

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. by subl.

Melting Point: Mp 121-122°

Aldrich: 29018-1

>>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%

Physical Description: Liq.

Boiling Point: Bp 200°. Bp₄₆ 103-105°

>>Derivative: Chloride

CAS Registry Number: 129714-97-2

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%

Refractive Index: n_D^{20} 1.5031

Aldrich: 29025-4

Other: Oakwood 2113

>>Derivative: Nitrile

Synonym(s): 1-Cyano-3,5-difluorobenzene

CAS Registry Number: 64248-63-1

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 83-85°

Aldrich: 29020-3

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 1136B; 1536C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1332A; 1419A, (*ir*)

Roe, A. *et al.*, *J.O.C.*, 1955, **20**, 1577, (*synth, deriv*)

Kruse, L.I. *et al.*, *J. Med. Chem.*, 1986, **29**, 887, (*synth, deriv*)