



>>Entry Name: 2,5-Difluorobenzoic acid

CAS Registry Number: 2991-28-8

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. ($CHCl_3$)

Melting Point: Mp 125-128°

Aldrich: 24802-9

>>Derivative: Chloride

CAS Registry Number: 35730-09-7

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: Bp_{15} 74-78°

Aldrich: 25936-5

>>Derivative: Amide

CAS Registry Number: 85118-03-2

Molecular Formula: $C_7H_5F_2NO$

Molecular Weight: 157.119

Accurate Mass: 157.03392

Percentage Composition: C 53.51%; H 3.21%; F 24.18%; N 8.91%; O 10.18%

Melting Point: Mp 114-116°

Other: Oakwood 1933

>>Derivative: Nitrile

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

CAS Registry Number: 64248-64-2

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: No phys. props. recorded

Aldrich: 24803-7

References:

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Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 210C; 350A; 456B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1331A; 1417D, (*ir*)

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

Kerr, C.A. *et al.*, *Aust. J. Chem.*, 1980, **33**, 2627, (*synth, deriv, ir, nmr*)

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

Morrow, G.W. *et al.*, *J.O.C.*, 1987, **52**, 713, (*synth*)

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