



>>Entry Name: 3,4-Difluorobenzoic acid

CAS Registry Number: 455-86-7

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. ( $H_2O$ )

Melting Point: Mp 119-120°

Aldrich: 26431-8

Fluka: 36885

>>Derivative: Me ester

Molecular Formula:  $C_8H_6F_2O_2$

Molecular Weight: 172.131

Accurate Mass: 172.033586

Percentage Composition: C 55.82%; H 3.51%; F 22.07%; O 18.59%

Physical Description: Cryst.

Melting Point: Mp 23.5°

Boiling Point: Bp<sub>23</sub> 69°

>>Derivative: Chloride

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<sub>15</sub> 61-63°

>>Derivative: Nitrile

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

CAS Registry Number: 64248-62-0

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 52-54°

Aldrich: 26433-4

#### References:

*Aldrich Library of  $^{13}C$  and  $^1H$  FT NMR Spectra*, 1992, **2**, 1104C; 1531A, (*nmr*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1330C; 1416C, (*ir*)

Minor, J.T. *et al.*, *J.O.C.*, 1952, **17**, 1425, (*synth, deriv*)

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

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

Suzuki, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1990, **63**, 2010, (*nitrile*)