



>>Entry Name: 3,4-Dichlorobenzoic acid

CAS Registry Number: 51-44-5

Molecular Formula:  $C_7H_4Cl_2O_2$

Molecular Weight: 191.013

Accurate Mass: 189.958834

Percentage Composition: C 44.02%; H 2.11%; Cl 37.12%; O 16.75%

Physical Description: Needles (EtOH aq. or  $C_6H_6$ )

Melting Point: Mp 208-209°

pKa Value:  $pK_a$  3.64 (25°)

Aldrich: 14493-2

Fluka: 35315

>>Derivative: Me ester

CAS Registry Number: 2905-68-2

Molecular Formula:  $C_8H_6Cl_2O_2$

Molecular Weight: 205.04

Accurate Mass: 203.974484

Percentage Composition: C 46.86%; H 2.95%; Cl 34.58%; O 15.61%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 45-47°

Rare Chemicals Library: S63497-2

>>Derivative: Chloride

CAS Registry Number: 3024-72-4

Molecular Formula:  $C_7H_3Cl_3O$

Molecular Weight: 209.458

Accurate Mass: 207.924946

Percentage Composition: C 40.14%; H 1.44%; Cl 50.78%; O 7.64%

Melting Point: Mp 15-18°

Boiling Point:  $Bp_{42}$  153-155°.  $Bp_1$  88-88.3°

Aldrich: 11194-5

Fluka: 35426

>>Derivative: Hydrazide

CAS Registry Number: 28036-91-1

Physical Description: Solid (EtOH)

Melting Point: Mp 167-168°

Other: MG Z1980

#### References:

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 210B; 349C, (*ir*)

*Aldrich Library of  $^{13}C$  and  $^1H$  FT NMR Spectra*, 1992, **2**, 1106B; 1347C, (*nmr*)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1393D, (*ir*)

*Aldrich Library of IR Spectra*, 2nd Ed., 848B, (*ir*)

*Aldrich Library of NMR Spectra*, **6**, 160C, (*pmr*)

Long, R.S., *J.A.C.S.*, 1947, **69**, 990

Ross, S.D., *J.A.C.S.*, 1948, **70**, 4039, (*synth, uv*)

Woodburn, H.M. *et al.*, *J.A.C.S.*, 1949, **71**, 1709

Yale, H.L. *et al.*, *J.A.C.S.*, 1953, **75**, 1933, (*hydrazide*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, DER600