



>>Entry Name: 3,5-Dichlorobenzoic acid

CAS Registry Number: 51-36-5

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.)

Melting Point: Mp 188°

pKa Value: pK_a 3.54 (22°)

Aldrich: D5750-7

Fluka: 35321

>>Derivative: Me ester

CAS Registry Number: 2905-67-1

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. (EtOH)

Melting Point: Mp 58°

Rare Chemicals Library: S74626-6

Supelco: R47-4290

>>Derivative: Et ester

CAS Registry Number: 91085-56-2

Molecular Formula: $C_9H_8Cl_2O_2$

Molecular Weight: 219.066

Accurate Mass: 217.990134

Percentage Composition: C 49.35%; H 3.68%; Cl 32.37%; O 14.61%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 37°

>>Derivative: Chloride

CAS Registry Number: 2905-62-6

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%

Boiling Point: Bp_{25} 135-137°

Refractive Index: n_D^{20} 1.5820

Aldrich: 29628-7

>>Derivative: Nitrile

Synonym(s): 1,3-Dichloro-5-cyanobenzene. 3,5-Dichlorobenzonitrile

CAS Registry Number: 6575-00-4

Molecular Formula: $C_7H_3Cl_2N$

Molecular Weight: 172.013

Accurate Mass: 170.964253

Percentage Composition: C 48.88%; H 1.76%; Cl 41.22%; N 8.14%

Melting Point: Mp 64-66°

Aldrich: 13939-4

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1137A; 1350B, (nmr)

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Asinger, F., *Monatsh. Chem.*, 1933, **62**, 344

Muller, E. *et al.*, *Ber.*, 1941, **74**, 807, (uv)

Jones, B. *et al.*, *J.C.S.*, 1955, 3845