



>>Entry Name: 2,4,6-Trichlorobenzoic acid

CAS Registry Number: 50-43-1

Molecular Formula: $C_7H_3Cl_3O_2$

Molecular Weight: 225.458

Accurate Mass: 223.919861

Percentage Composition: C 37.29%; H 1.34%; Cl 47.17%; O 14.19%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 164°

Aldrich: 34428-1

>>Derivative: Me ester

Molecular Formula: $C_8H_5Cl_3O_2$

Molecular Weight: 239.484

Accurate Mass: 237.935511

Percentage Composition: C 40.12%; H 2.10%; Cl 44.41%; O 13.36%

Physical Description: Cryst.

Melting Point: Mp 43-44° (40-43°)

>>Derivative: Chloride

CAS Registry Number: 4136-95-2

Molecular Formula: $C_7H_2Cl_4O$

Molecular Weight: 243.903

Accurate Mass: 241.885973

Percentage Composition: C 34.47%; H 0.83%; Cl 58.14%; O 6.56%

Physical Description: Oil

Boiling Point: Bp 275°

Aldrich: 34550-4

>>Derivative: Amide

CAS Registry Number: 23400-04-6

Molecular Formula: $C_7H_4Cl_3NO$

Molecular Weight: 224.473

Accurate Mass: 222.935845

Percentage Composition: C 37.46%; H 1.80%; Cl 47.38%; N 6.24%; O 7.13%

Physical Description: Cryst.

Melting Point: Mp 181°

>>Derivative: Nitrile

Synonym(s): 2,4,6-Trichlorobenzonitrile. 1,3,5-Trichloro-2-cyanobenzene

CAS Registry Number: 6575-05-9

Molecular Formula: $C_7H_2Cl_3N$

Molecular Weight: 206.458

Accurate Mass: 204.92528

Percentage Composition: C 40.72%; H 0.98%; Cl 51.52%; N 6.78%

Physical Description: Needles

Melting Point: Mp 77.5°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 1141C; 1352A, (*nmr*)

Sudborough, J.J., *J.C.S.*, 1895, 601, (*synth*)

Cohen, J.B. *et al.*, *J.C.S.*, 1902, 1336, (*synth*)

Kirkland, J.J., *Anal. Chem.*, 1961, **33**, 1520, (*glc*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1981, **9**, 478; **11**, 552; **16**, 353, (*use, chloride*)

Castaner, J. *et al.*, *J.O.C.*, 1991, **56**, 103, (*synth, ir*)

Lalancette, R.A. *et al.*, *Acta Cryst. C*, 1996, **52**, 1801, (*cryst struct*)