



>>Entry Name: 2,5-Dichlorobenzoic acid

CAS Registry Number: 50-79-3

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%

Melting Point: Mp 155.5°

pKa Value: pK_a 2.47 (25°)

Hazard & Toxicity: LD₅₀ (mus, scu) 1200 mg/kg

Aldrich: 14494-0

Fluka: 35301

>>Derivative: Me ester

CAS Registry Number: 2905-69-3

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%

Melting Point: Mp 37-40°

Aldrich: 16673-1

>>Derivative: Et ester

CAS Registry Number: 35112-27-7

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%

Boiling Point: Bp 271°

Density: d^0 1.328

>>Derivative: Chloride

CAS Registry Number: 2905-61-5

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: Bp₁ 95.3-95.5°

>>Derivative: Amide

CAS Registry Number: 5980-26-7

Molecular Formula: $C_7H_5Cl_2NO$

Molecular Weight: 190.028

Accurate Mass: 188.974818

Percentage Composition: C 44.24%; H 2.65%; Cl 37.31%; N 7.37%; O 8.42%

Melting Point: Mp 155°

>>Derivative: Nitrile

Synonym(s): 1,4-Dichloro-2-cyanobenzene

CAS Registry Number: 21663-61-6

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%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 129-130°

Rare Chemicals Library: S38986-2

References: