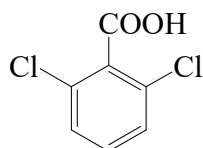




>>Entry Name: 2,6-Dichlorobenzoic acid



CAS Registry Number: 50-30-6

Molecular Formula: C₇H₄Cl₂O₂

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), prisms (H₂O or C₆H₆)

Melting Point: Mp 144°

pKa Value: pK_a 1.59 (25°) pK_a 1.82 (25°, H₂O)

Hazard & Toxicity: LD₅₀ (mus, scu) 1500 mg/kg

Aldrich: D5745-0

Fluka: 35310

Sigma: D1541

>>Derivative: Et ester

CAS Registry Number: 81055-73-4

Molecular Formula: C₉H₈Cl₂O₂

Molecular Weight: 219.066

Accurate Mass: 217.990134

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

Physical Description: Oil

>>Derivative: Chloride

CAS Registry Number: 4659-45-4

Molecular Formula: C₇H₃Cl₃O

Molecular Weight: 209.458

Accurate Mass: 207.924946

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

Boiling Point: Bp₁₈ 126-128°

Hazard & Toxicity: Lachrymator

Aldrich: 18751-8

Fluka: 35423

Sigma: D1291

>>Derivative: Amide

CAS Registry Number: 2008-58-4

Molecular Formula: C₇H₅Cl₂NO

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 198°

Aldrich: 14183-6

>>Derivative: Nitrile

Synonym(s): 1,3-Dichloro-2-cyanobenzene. 2,6-Dichlorobenzonitrile, 9Cl. Dichlobenil, ANSI, BSI, ISO, WSSA. DBN, JMAF. Casoron. Decabane. Prefix D. Silbenil

CAS Registry Number: 1194-65-6

Molecular Formula: C₇H₃Cl₂N

Molecular Weight: 172.013

Accurate Mass: 170.964253

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

Use/Importance: Herbicide. Cellulose biosynthesis inhibitor

Melting Point: Mp 142.5-143.5°

Hazard & Toxicity: LD₅₀ (rat, orl) 2710 mg/kg. LD₅₀ (rbt, skn) 1350 mg/kg

Aldrich: D5755-8

Fluka: 35380