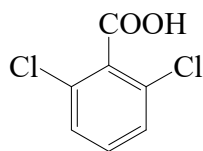




>>Entry Name: 2,6-Dichlorobenzoic acid



**CAS Registry Number:** 50-30-6

**Molecular Formula:** C<sub>7</sub>H<sub>4</sub>Cl<sub>2</sub>O<sub>2</sub>

**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 (H<sub>2</sub>O or C<sub>6</sub>H<sub>6</sub>)

**Melting Point:** Mp 144°

**pKa Value:** pK<sub>a</sub> 1.59 (25°) pK<sub>a</sub> 1.82 (25°, H<sub>2</sub>O)

**Hazard & Toxicity:** LD<sub>50</sub> (mus, scu) 1500 mg/kg

**Aldrich:** D5745-0

**Fluka:** 35310

**Sigma:** D1541

>>Derivative: Et ester

**CAS Registry Number:** 81055-73-4

**Molecular Formula:** C<sub>9</sub>H<sub>8</sub>Cl<sub>2</sub>O<sub>2</sub>

**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:** C<sub>7</sub>H<sub>3</sub>Cl<sub>3</sub>O

**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<sub>18</sub> 126-128°

**Hazard & Toxicity:** Lachrymator

**Aldrich:** 18751-8

**Fluka:** 35423

**Sigma:** D1291

>>Derivative: Amide

**CAS Registry Number:** 2008-58-4

**Molecular Formula:** C<sub>7</sub>H<sub>5</sub>Cl<sub>2</sub>NO

**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:** C<sub>7</sub>H<sub>3</sub>Cl<sub>2</sub>N

**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:** LD<sub>50</sub> (rat, orl) 2710 mg/kg. LD<sub>50</sub> (rbt, skn) 1350 mg/kg

**Aldrich:** D5755-8

**Fluka:** 35380