

# Benzyl chloride CAS number 100-44-7

TAJBNZ-CCWHYM550

Taj Active Pharmaceuticals Ingredients

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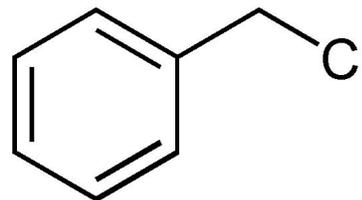


Raw Material / Chemicals Index

## BENZYL CHLORIDE

### **IDENTIFICATION**

CAS NO. 100-44-7  
BENZYL CHLORIDE EINECS NO. 202-853-6  
FORMULA C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>Cl  
MOL WT. 126.59  
H.S. CODE 2903.69  
TOXICITY Oral rat LD50: 1231 mg/kg



### **CHEMICAL PROPERTIES**

#### **PHYSICAL STATE : Clear to yellow liquid**

MELTING POINT -39 C  
BOILING POINT 179 C  
SPECIFIC GRAVITY 1.10  
SOLUBILITY IN WATER : Reacts slowly  
SOLVENT SOLUBILITY : Soluble in most common organic solvents(alcohol, chloroform, ether)  
pH  
VAPOR DENSITY : 4.4  
AUTOIGNITION : 585 C NFPA RATINGS Health: 3 Flammability: 2 Reactivity: 1  
REFRACTIVE INDEX : 1.5415  
FLASH POINT 67 C  
STABILITY :Unstable. Inhibitors must be used to prevent polymerization.(propylene oxide, sodium carbonate, lime, or trimethylamine )  
Vapour density: 4.36 (air=1)  
Vapour pressure: 1 mm Hg at 20 C Explosion limits: 1.1% (lower), 7.1% (upper) Viscosity: 1.3 centistokes at 25 C  
Critical temperature: 411 C

#### Toxicology

Toxic. Probable human carcinogen. Contact with the eyes may cause permanent damage. Harmful by inhalation, ingestion and through skin contact. Corrosive - causes burns. May cause CNS depression. UK STEL (EH40/2000) 1.5 ppm. UK MEL 8h TWA (EH40/2000) 0.5 ppm.

#### **Toxicity data**

ORL-RAT LD50 1231 mg kg-1  
IHL-RAT LD50 150 ppm/2h.  
SCU-RAT LD50 1000 mg/kg.  
ORL-MAM LD50 1500 mg kg-1Risk phrases R22 R23 R37 R38 R40 R41 R45 R48.

### **Personal protection**

Safety glasses, gloves, good ventilation. Treat as a potential carcinogen.

### **Preparation**

Benzyl chloride, or  $\alpha$ -chlorotoluene, is an organic compound consisting of a phenyl group substituted with a chloromethyl group.

Benzyl chloride can be prepared by free radical chlorination of toluene or the Blanc chloromethylation of benzene. Benzyl chloride is also easily prepared by mixing benzyl alcohol with a large molar excess of concentrated hydrochloric acid.

### **Uses**

**Benzyl chloride** is used in organic synthesis for the introduction of the benzyl protecting group for alcohols (yielding the corresponding benzyl ether) and carboxylic acids (yielding the corresponding benzyl ester).

It may be used in the synthesis of amphetamine-class drugs, and for this reason sales of benzyl chloride are monitored as a List II drug precursor chemical by the Drug Enforcement Administration

Benzyl chloride reacts with water in a hydrolysis reaction to form benzyl alcohol and hydrogen chloride. When the latter is dissolved in water, it forms hydrochloric acid. Since benzyl chloride is quite volatile at room temperature, it can easily reach the mucous membranes where the hydrolysis takes place with production of hydrochloric acid.

This explains why benzyl chloride is a lachrymator and has been used as a war gas. It is also very irritating to the skin. Benzyl chloride also reacts readily with metallic magnesium to produce a Grignard Reagent, although the resulting benzyl magnesium chloride tends to dimerize due to the stability of the benzyl radical. This makes the use of benzyl Grignard reagents unfavorable.

### **Data Reported and Evaluation**

#### **Human data**

Occupational exposure to benzyl chloride may occur during its manufacture and during its use in the production of benzyl phthalates, benzyl alcohol, quaternary ammonium salts, pharmaceuticals and benzyl esters; but no data were available on levels of exposure.

No data were available to assess the mutagenicity or teratogenicity of this compound to man.

No case report or epidemiological study involving exposure to benzyl chloride alone was available to the Working Group. Six cases of respiratory cancer have been reported among benzoyl chloride manufacturing workers in two small plants, who were also potentially exposed to benzyl chloride.

The cases occurred in relatively young workers, three of whom were nonsmokers.

#### **Evaluation**

There is limited evidence that benzyl chloride is carcinogenic in experimental animals.

Although the epidemiological data were inadequate to evaluate the carcinogenicity of benzyl chloride alone, they provide limited evidence that employment in the production of benzoyl chloride and its chlorinated toluene precursors, which involves exposure to benzyl chloride, represents a carcinogenic risk to man.

### **SALES SPECIFICATION**

**APPEARANCE: Clear liquid**

**ASSAY: 99.5% min**

**SPECIFIC GRAVITY: 1.10**

**COLOUR, APHA 25 max**

**STABILIZER: 0.02% on request**

TRANSPORTATION

**PACKING**

**220kg in drum**

**HAZARD CLASS 6.1, 8 (Packing Group: II)  
UN NO. 1738**

**Hazard Symbols: T, Risk Phrases: 45-22-23-37/38-41-48/22, Safety Phrases: 53-45**

**WARNING:  
THIS PRODUCT CONTAINS A CHEMICAL(S) KNOWN TO CAUSE  
CANCER.**

**NFPA Ratings: Health: 3 Flammability: 2 Reactivity: 1**

Origin: INDIA

We have experience in Exporting and Manufacturing of all Countries and Overseas medicines in quick reliable manner and we are very interested to start collaboration with your company or organisation!



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**Label Hazard Warning:**

DANGER! CORROSIVE. CAUSES BURNS TO ANY AREA OF CONTACT. HARMFUL IF SWALLOWED OR INHALED. CAUSES SEVERE IRRITATION TO EYES, SKIN AND RESPIRATORY TRACT. AFFECTS CENTRAL NERVOUS SYSTEM. COMBUSTIBLE LIQUID AND VAPOR.

**Label Precautions:**

Do not get in eyes, on skin, or on clothing.

Do not breathe mist.

Keep container closed.

Use only with adequate ventilation.

Wash thoroughly after handling.

Keep away from heat and flame.

**Label First Aid:**

If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. In case of contact, wipe off excess material from skin then immediately flush eyes or skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. If swallowed, DO NOT INDUCE VOMITING. Give large quantities of water. Never give anything by mouth to an unconscious person. In all cases get medical attention immediately.