

Benzyl chloride Cas No. 100-44-7

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

Active Pharmaceuticals Ingredients Manufacturers



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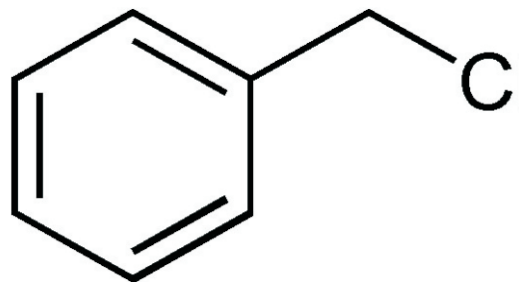
Taj Pharmaceuticals Ltd.

Benzyl chloride

CAS No. : 100-44-7

**IDENTIFICATION**

CAS NO. 100-44-7
 BENZYL CHLORIDE EINECS NO. 202-853-6
 FORMULA C₆H₅CH₂Cl
 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-1 Risk phrases R22 R23 R37 R38 R40 R41 R45 R48.

Personal protection

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



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Benzyl Chloride

CAS Number 100-44-7



Preparation

Benzyl chloride, or α -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.

Detail icon



Note /Government Notification: These chemicals are designated as those that are used in the manufacture of the controlled substances and are important to the manufacture of the substances. For any (Control Substance) products Import and Export *** subjected to your country government laws /control substance ACT.

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The Controlled Substances Act (CSA) was enacted into law by the Congress of the United States as Title II of the Comprehensive Drug Abuse Prevention and Control Act of 1970.[1] The CSA is the federal U.S. drug policy under which the manufacture, importation, possession, use and distribution of certain substances is regulated. The Act also served as the national implementing legislation for the Single Convention on Narcotic Drugs

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This leaflet was prepared by
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