# **Chemical Book India**

Chemical	Safety	<b>Data Sheet</b>	MSDS / SDS
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# a-chlorotoluene SDS

Revision Date: 2024-04-25 Revision Number: 1

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# SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier	
Product name:	a-chlorotoluene
CAS:	100-44-7

## Relevant identified uses of the substance or mixture and uses advised against

 Relevant identified
 For R&D use only. Not for medicinal, household or other use.

 uses:
 uses advised

 uses:
 none

 against:

## **Company Identification**

Company:	Chemicalbook.in
Address:	5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090
Telephone:	+91 9550333722

# **SECTION 2: Hazards identification**

## Classification of the substance or mixture

Acute toxicity - Category 4, Oral Skin irritation, Category 2

Serious eye damage, Category 1 Acute toxicity - Category 3, Inhalation Specific target organ toxicity - single exposure, Category 3 Carcinogenicity, Category 1B Specific target organ toxicity - repeated exposure, Category 2

## GHS label elements, including precautionary statements

Pictogram(s)



Signal word Danger

## Hazard statement(s)

H302 Harmful if swallowed H315 Causes skin irritation H318 Causes serious eye damage H331 Toxic if inhaled H335 May cause respiratory irritation H350 May cause cancer H373 May cause damage to organs through prolonged or repeated exposure

# Precautionary statement(s)

## Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P203 Obtain, read and follow all safety instructions before use.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.

# Response

P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P321 Specific treatment (see ... on this label).
P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P316 Get emergency medical help immediately.
P319 Get medical help if you feel unwell.
P318 IF exposed or concerned, get medical advice.

#### Storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up.

### Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

## Other hazards which do not result in classification

no data available

# SECTION 3: Composition/information on ingredients

Substance

Chemical name:	a-chlorotoluene
Common names and synonyms:	a-chlorotoluene
CAS number:	100-44-7
EC number:	202-853-6
Concentration:	100%

# **SECTION 4: First aid measures**

Description of necessary first-aid measures

### If inhaled

Fresh air, rest. Half-upright position. Refer for medical attention.

#### Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

#### Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

## Following ingestion

Rinse mouth. Refer for medical attention .

## Most important symptoms/effects, acute and delayed

Intensely irritating to skin, eyes, and mucous membranes. Highly toxic; may cause death or permanent injury after very short exposure to small quantities. Has been listed as a direct-acting or primary carcinogen. Large doses cause central nervous system depression. (EPA, 1998)

### Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aromatic hydrocarbons and related compounds

# **SECTION 5: Firefighting measures**

## Suitable extinguishing media

Use water spray, dry chemical, foam, or carbon dioxide. Use water to keep fire-exposed containers cool. Approach fire from upwind to avoid hazardous vapors and toxic decomposition products.

## Specific hazards arising from the chemical

It burns but does not ignite readily. It may ignite combustibles. When heated to decomposition, it emits toxic and corrosive fumes. Some organic chlorides decompose to yield phosgene. Incompatible with active metals such as copper, aluminum, magnesium, iron, zinc, and tin and keep from strong oxidizing agents. Avoid contact with acids or acid fumes. Keep separate from oxidizing materials. May become unstable at elevated temperatures and pressures; may react with water resulting in some nonviolent release of energy. Polymerizes with evolution of heat and hydrogen chloride when in contact with all common metals except nickel and lead. (EPA, 1998)

#### Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

# **SECTION 6: Accidental release measures**

#### Personal precautions, protective equipment and emergency procedures

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in covered non-metallic containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

#### Environmental precautions

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in covered non-metallic containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

#### Methods and materials for containment and cleaning up

Environmental considerations: Air spill: Apply water spray or mist to knock down vapors. Vapor knockdown water is corrosive or toxic and should be diked for containment.

# SECTION 7: Handling and storage

#### Precautions for safe handling

NO open flames. Above 67°C use a closed system and ventilation. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

#### Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs and incompatible materials. See Chemical Dangers. Dry. Ventilation along the floor. Store only if stabilized. Separated from food and feedstuffs and incompatible materials . Ventilation along the floor. Store only if stabilized.

# SECTION 8: Exposure controls/personal protection

**Control parameters** 

# Occupational Exposure limit values

MAK: skin absorption (H); carcinogen category: 2

## Biological limit values

no data available

# Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

# Individual protection measures, such as personal protective equipment (PPE)

## Eye/face protection

Wear safety goggles or eye protection in combination with breathing protection.

# Skin protection

Protective gloves. Protective clothing.

# **Respiratory protection**

Use ventilation, local exhaust or breathing protection.

# Thermal hazards

no data available

# SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Colorless.
Odour:	Rather unpleasant, irritating odor

Melting point/freezing point:	>= -48 - <= -43 °C.
Boiling point or initial boiling point and boiling range:	179.4 °C. Atm. press.:101.3 kPa.
Flammability:	Class IIIA Combustible Liquid: Fl.P. at or above 140°F and below 200°F.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 1.1% by volume; Upper flammable limit: 7.1% by volume
Flash point:	67 °C. Atm. press.:1 atm.
Auto-ignition temperature:	585 °C. Atm. press.:1 013 hPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 1.501. Temperature:15.0°C.;dynamic viscosity (in mPa s) = 1.38. Temperature:20°C.;dynamic viscosity (in mPa s) = 1.289. Temperature:25.0°C.
Solubility:	Insoluble in water
<b>B</b>	
Partition coefficient n- octanol/water:	log Pow = 2.3. Temperature:20 $^{\circ}$ C. Remarks:Information on temperature and pH was not available in the article.
coefficient n-	ě 1
coefficient n- octanol/water:	available in the article. 0.16 kPa. Temperature:25 °C.;0.747 kPa. Temperature:50 °C.;2.66 kPa. Temperature:75
coefficient n- octanol/water: Vapour pressure: Density and/or	available in the article. 0.16 kPa. Temperature:25 °C.;0.747 kPa. Temperature:50 °C.;2.66 kPa. Temperature:75 °C.

# SECTION 10: Stability and reactivity

## Reactivity

The substance polymerizes under the influence of all common metals except nickel and lead. This produces corrosive fumes (hydrogen chloride - see ICSC 0163). This generates fire or explosion hazard. On combustion, forms toxic and corrosive fumes of hydrogen chloride. Reacts vigorously with strong oxidants. Attacks many metals in the presence of water.

# Chemical stability

Stablity during transport: stable

## Possibility of hazardous reactions

Combustible. Gives off irritating or toxic fumes (or gases) in a fire. Halogenated aliphatic compounds, such as BENZYL CHLORIDE, are moderately or very reactive. Halogenated organics generally become less reactive as more of their hydrogen atoms are replaced with halogen atoms. Materials in this group are incompatible with strong oxidizing and reducing agents. Also, they are incompatible with many amines, nitrides, azo/diazo compounds, alkali metals, and epoxides.

## Conditions to avoid

no data available

# Incompatible materials

Will react with water or steam to produce toxic and corrosive fumes /HCl and chlorine gas/; can react vigorously with oxidizing materials.

# Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /hydrogen chloride/.

# SECTION 11: Toxicological information

Acute toxicity Oral: LD50 Mouse oral 1500 mg/kg Inhalation: LC50 - rat (male) - 0.74 mg/L air. Dermal: LD50 - (male/female) - > 794 - < 1 000 mg/kg bw.

#### Skin corrosion/irritation

no data available

#### Serious eye damage/irritation

no data available

#### Respiratory or skin sensitization

no data available

### Germ cell mutagenicity

no data available

## Carcinogenicity

Evaluation: There is limited evidence in humans for the carcinogenicity of alpha-chlorinated toluenes and benzoyl chloride. There is sufficient evidence in experimental animals for the carcinogenicity of benzyl chloride. ... Overall evaluation: Combined exposures to alpha-chlorinated toluenes and benzoyl chloride are probably carcinogenic to humans (Group 2A). alpha-Chlorinated toluenes & benzoyl chloride

## Reproductive toxicity

No studies were located regarding developmental or reproductive effects in humans from benzyl chloride exposure. (-) One animal study showed an increase in embryonal mortality, along with retarded development of the offspring in rats given benzyl chloride orally.

## STOT-single exposure

The substance is corrosive to the eyes. The vapour is irritating to the eyes, skin and respiratory tract. Inhalation of the vapour or aerosol may cause lung oedema. See Notes. The substance may cause effects on the central nervous system. This may result in unconsciousness.

## STOT-repeated exposure

The substance may have effects on the liver and kidneys. This may result in tissue lesions. This substance is possibly carcinogenic to humans. Animal tests show that this substance possibly causes toxicity to human reproduction or development.

#### Aspiration hazard

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at  $20^{\circ}$ C , on spraying much faster.

# **SECTION 12: Ecological information**

#### Toxicity

Toxicity to fish: LC50 - Brachydanio rerio and Leuciscus idus - 4 mg/L - 96 h. Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 6.1 mg/L - 48 h. Toxicity to algae: Toxicity threshold (similar to EC3) - Microcystis aeruginosa and Scenedesmus quadricauda - 30 mg/L - 8 d. Toxicity to microorganisms: toxicity threshold - Pseudomonas putida - 4.8 mg/L - 16 h.

#### Persistence and degradability

AEROBIC: Benzyl chloride, present at 100 mg/L, reached 70.9% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(1). Benzyl chloride biodegraded readily with the formation of dechlorinated products during a 2-day incubation period using raw sewage and raw sewage acclimated to non-chlorinated compounds(2). However, since benzyl chloride is subject to hydrolysis(3-5), it is probably the biodegradation of benzyl alcohol that is measured in these studies(SRC).

#### Bioaccumulative potential

An estimated BCF of 20 was calculated in fish for benzyl chloride(SRC), using a log Kow of 2.30(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

#### Mobility in soil

The Koc of benzyl chloride is estimated as 100(SRC), using a log Kow of 2.30(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that benzyl chloride is expected to have high mobility in soil.

#### Other adverse effects

no data available

# **SECTION 13: Disposal considerations**

## Disposal methods

## Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

## Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

# SECTION 14: Transport information

## **UN Number**

ADR/RID: UN1738 (For reference only, please check.) IMDG: UN1738 (For reference only, please check.) IATA: UN1738 (For reference only, please check.)

# **UN Proper Shipping Name**

ADR/RID: BENZYL CHLORIDE (For reference only, please check.) IMDG: BENZYL CHLORIDE (For reference only, please check.) IATA: BENZYL CHLORIDE (For reference only, please check.)

# Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.) IMDG: 6.1 (For reference only, please check.) IATA: 6.1 (For reference only, please check.)

# Packing group, if applicable

ADR/RID: II (For reference only, please check.) IMDG: II (For reference only, please check.) IATA: II (For reference only, please check.)

## Environmental hazards

ADR/RID: No IMDG: No IATA: No

## Special precautions for user

no data available

### Transport in bulk according to IMO instruments

no data available

# SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

## Korea Existing Chemicals List (KECL)

Listed.

# **SECTION 16: Other information**

## Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

## References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=O&request\_locale=en

CAWEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp ECHA - European Chemicals Agency, website: https://echa.europa.eu/

### Other Information

Depending on the degree of exposure, periodic medical examination is suggested. The symptoms of lung oedema often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation are therefore essential. Immediate administration of an appropriate inhalation therapy by a doctor, or by an authorized person, should be considered. An added stabilizer or inhibitor can influence the toxicological properties of this substance; consult an expert.

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