

## Chemical Safety Data Sheet MSDS / SDS

## 6-tert-butyl-2,4-xyleneol 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: 6-tert-butyl-2,4-xyleneol

CAS: 1879-09-0

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

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

Uses advised against: none

**Company Identification**

Company: Chemicalbook.in

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**SECTION 2: Hazards identification****Classification of the substance or mixture**

Acute toxicity - Category 4, Oral

Acute toxicity - Category 1, Dermal

Skin irritation, Category 2  
Eye irritation, Category 2  
Specific target organ toxicity - repeated exposure, Category 2  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

#### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

#### Hazard statement(s)

H302 Harmful if swallowed  
H310 Fatal in contact with skin  
H315 Causes skin irritation  
H319 Causes serious eye irritation  
H373 May cause damage to organs through prolonged or repeated exposure  
H411 Toxic to aquatic life with long lasting effects

#### Precautionary statement(s)

#### Prevention

P264 Wash ... thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P262 Do not get in eyes, on skin, or on clothing.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P273 Avoid release to the environment.

#### Response

P301+P317 IF SWALLOWED: Get medical help.  
P330 Rinse mouth.  
P302+P352 IF ON SKIN: Wash with plenty of water/...  
P316 Get emergency medical help immediately.  
P321 Specific treatment (see ... on this label).  
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.  
P332+P317 If skin irritation occurs: Get medical help.  
P362+P364 Take off contaminated clothing and wash it before reuse.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P319 Get medical help if you feel unwell.  
P391 Collect spillage.

#### **Storage**

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:	6-tert-butyl-2,4-xyleneol
Common names and synonyms:	6-tert-butyl-2,4-xyleneol
CAS number:	1879-09-0
EC number:	217-533-1
Concentration:	100%

### **SECTION 4: First aid measures**

#### **Description of necessary first-aid measures**

##### **If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

##### **Following skin contact**

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### **Following eye contact**

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### **Following ingestion**

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

#### **Most important symptoms/effects, acute and delayed**

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: TOXIC; inhalation, ingestion or skin contact with material may cause severe injury or death. Contact with molten substance may cause severe burns to skin and eyes. Avoid any skin contact. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

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

no data available

## **SECTION 5: Firefighting measures**

#### **Suitable extinguishing media**

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: SMALL FIRE: Dry chemical, CO2 or water spray. LARGE FIRE: Dry chemical, CO2, alcohol-resistant foam or water spray. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal; do not scatter the material. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. (ERG, 2016)

#### **Specific hazards arising from the chemical**

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)

### **Special protective actions for fire-fighters**

Wear self-contained breathing apparatus for firefighting if necessary.

## **SECTION 6: Accidental release measures**

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

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

## **SECTION 7: Handling and storage**

### **Precautions for safe handling**

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**

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

## **SECTION 8: Exposure controls/personal protection**

### **Control parameters**

### **Occupational Exposure limit values**

no data available

### **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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### **Skin protection**

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### **Respiratory protection**

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

#### **Thermal hazards**

no data available

## **SECTION 9: Physical and chemical properties and safety characteristics**

Physical state:	Liquid. Viscous.
Colour:	Colourless to yellow-orange.
Odour:	no data available
Melting point/freezing point:	-6 °C. Remarks:Atm. pressure, Decomposition and Sublimation within the study report. Assumed to be conducted at ATP.

Boiling point or initial boiling point and boiling range:	248 °C. Atm. press.:100.6 kPa.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	111 °C. Atm. press.:101 kPa.
Auto-ignition temperature:	364 °C. Atm. press.:101 kPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 50. Temperature:20°C.;kinematic viscosity (in mm <sup>2</sup> /s) = 50. Temperature:20°C.
Solubility:	In water: 0.12 g/L. Temperature:20 °C. Remarks:PH in the study report.
Partition coefficient n-octanol/water:	log Pow = 3.64. Temperature:35 °C. Remarks:PH in the study report.;Pow = 4 340. Temperature:35 °C. Remarks:PH in the study report.
Vapour pressure:	4.2 Pa. Temperature:25 °C. Remarks:The test item did not change in appearance under the conditions used in the determination.
Density and/or relative density:	0.967. Temperature:20 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

#### **Chemical stability**

no data available

#### **Possibility of hazardous reactions**

Phenols, such as 2,4-DIMETHYL-6-TERT-BUTYL PHENOL, do not behave as organic alcohols, as one might guess from the presence of a hydroxyl (-OH) group in their structure. Instead, they react as weak organic acids. Phenols and cresols are much weaker as acids than common carboxylic acids (phenol has  $pK_a = 9.88$ ). These materials are incompatible with strong reducing substances such as hydrides, nitrides, alkali metals, and sulfides. Flammable gas ( $H_2$ ) is often generated, and the heat of the reaction may ignite the gas. Heat is also generated by the acid-base reaction between phenols and bases. Such heating may initiate polymerization of the organic compound. Phenols are sulfonated very readily (for example, by concentrated sulfuric acid at room temperature). The reactions generate heat. Phenols are also nitrated very rapidly, even by dilute nitric acid. Nitrated phenols often explode when heated. Many of them form metal salts that tend toward detonation by rather mild shock.

#### **Conditions to avoid**

no data available

#### **Incompatible materials**

no data available

#### **Hazardous decomposition products**

no data available

### **SECTION 11: Toxicological information**

#### **Acute toxicity**

Oral: no data available

Inhalation: no data available

Dermal: no data available

#### **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**

no data available

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

**SECTION 12: Ecological information**

**Toxicity**

Toxicity to fish: LC50 - *Oryzias latipes* - 2.5 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 2.9 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 6 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - > 10 - < 100 mg/L - 3 h.

Remarks: Respiration rate.

#### **Persistence and degradability**

no data available

#### **Bioaccumulative potential**

no data available

#### **Mobility in soil**

no data available

#### **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: no data available

IMDG: no data available

IATA: no data available

**UN Proper Shipping Name**

ADR/RID: no data available

IMDG: no data available

IATA: no data available

**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: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

**Environmental hazards**

ADR/RID: Yes

IMDG: Yes

IATA: Yes

**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

Not 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=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

CAMEO 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/>

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