

## Chemical Safety Data Sheet MSDS / SDS

**2,3,6-Trimethylphenol**

Revision Date:2024-08-17 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 2,3,6-Trimethylphenol  
CBnumber : CB0717010  
CAS : 2416-94-6  
EINECS Number : 219-330-3  
Synonyms : 2,3,6-trimethylphenol,3-Hydroxypseudocumene

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

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

Skin irritation, Category 2  
Skin sensitization, Sub-category 1B  
Serious eye damage, Category 1

**Label elements****Pictogram(s)**

☐

Signal word : Danger

**Hazard statement(s)**

H314 Causes severe skin burns and eye damage  
H315 Causes skin irritation  
H317 May cause an allergic skin reaction  
H318 Causes serious eye damage

**Precautionary statement(s)**

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P264 Wash hands thoroughly after handling.

P264 Wash skin thoroughly after handling.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P405 Store locked up.

P501 Dispose of contents/container to.....

#### **Prevention**

P264 Wash ... thoroughly after handling.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

#### **Response**

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.

P333+P317 If skin irritation or rash occurs: Get medical help.

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.

#### **Storage**

none

#### **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**

no data available

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## SECTION 3: Composition/information on ingredients

#### **Substance**

Product name	: 2,3,6-Trimethylphenol
Synonyms	: 2,3,6-trimethylphenol,3-Hydroxypseudocumene
CAS	: 2416-94-6
EC number	: 219-330-3
MF	: C9H12O
MW	: 136.19

## SECTION 4: First aid measures

### Description of 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 and effects, both acute and delayed

no data available

### Indication of any immediate medical attention and special treatment needed

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary. Monitor for shock and treat if necessary. Anticipate seizures and treat if necessary. For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport. Administer activated charcoal. Dilution may be contraindicated because it may increase absorption. Do not use emetics. Cover skin burns with dry sterile dressings after decontamination. Phenols and Related compounds

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## SECTION 5: Firefighting measures

### Extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

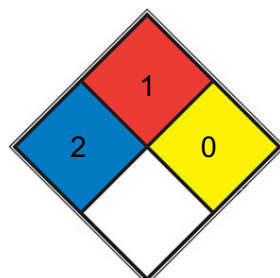
### Specific Hazards Arising from the Chemical

no data available

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### NFPA 704



Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl](#)

■ HEALTH 2  
[ether](#), ammonium phosphate, iodine)

Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion

■ FIRE 1 can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

□ SPEC.

□ HAZ.

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## 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.

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## 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.

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## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

## Exposure 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

### Eye/face protection

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

### Skin protection

Wear fire/flammable 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

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Physical state	Solid. Powder.
Colour	Yellow - orange.
Odour	no data available
Melting point/freezing point	60 - 62 °C.
Boiling point or initial boiling point and boiling range	226.5 °C. Atm. press.:1 000 hPa.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	104 °C. Atm. press.:1 013.25 hPa.
Auto-ignition temperature	405 °C. Atm. press.:1 013.25 hPa.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	dynamic viscosity (in mPa s) = 1.44. Temperature:70.0°C.;kinematic viscosity (in mm <sup>2</sup> /s) = 1.48. Temperature:70.0°C.
Solubility	methanol: 0.1 g/mL, clear
Partition coefficient n-octanol/water	log Pow = 2.72. Temperature:25 °C. Remarks:No data on pH value is reported.
Vapour pressure	0.02 hPa. Temperature:20 °C. Remarks:Extrapoliert.;0.037 hPa. Temperature:25 °C. Remarks:Interpolated.;0.56 hPa. Temperature:50 °C. Remarks:Interpolated.
Density and/or relative density	1.1. 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

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD50 - rat (male/female) - ca. 3 600 mg/kg bw. Remarks:After 7 days; 95% CL not given.
- Inhalation: discriminating conc. - rat (male/female) - > 0.59 mg/L air.
- Dermal: LD50 - rat - > 2 000 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

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster CHL/IU cells

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Test Guideline 473

Metabolic activation: with and without metabolic activation

Result:Structural chromosomal aberrations, including gaps, were induced at 200 µg/ mL on 6 hr short-term treatment with an S9 mix (11.5 %) and without an S9 mix (11.0 %), and at 50, 100 and 200 µg/ mL on 48 hr treatment (9.5, 13.5 and 8.5 %, respectively) in the

Test Type: Ames test

Test system: Salmonella typhimurium TA100, TA1535, TA98, TA1537, Escherichia coli WP2 uvrA

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Test Guidelines 471 and 472

Metabolic activation: with and without metabolic activation

Result:Negative

### **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

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## SECTION 12: Ecological information

### **Toxicity**

Toxicity to fish: LC50 - Pimephales promelas - 8.2 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 9.15 mg/L - 48 h.

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 19 mg/L - 72 h.

Toxicity to microorganisms: EC20 - activated sludge, domestic - ca. 80 mg/L - 30 min. Remarks:Respiration rate.

### **Persistence and degradability**

2,3,6-Trimethylphenol, at an initial concentration of 0.37 mg/l, underwent no degradation when incubated in coal tar-contaminated groundwater in an anaerobic digester for 8 weeks(1).

### **Bioaccumulative potential**

An estimated BCF of 60 was calculated for 2,3,6-trimethylphenol(SRC), using a log Kow of 2.67(1) and a regression-derived equation(2).

According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(SRC).

### **Mobility in soil**

The Koc of 2,3,6-trimethylphenol is estimated as 700(SRC), using a log Kow of 2.67(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 2,3,6-trimethylphenol is expected to have low mobility in soil(SRC).

### **Other adverse effects**

no data available

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## 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.

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## SECTION 14: Transport information

### UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (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

Not Listed.

#### New Zealand Inventory of Chemicals (NZIoC)

Listed.

#### PICCS

Listed.

#### Vietnam National Chemical Inventory

Listed.

#### IECSC

Listed.

#### Korea Existing Chemicals List (KECL)

Not Listed.

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## 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?pagenID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pagenID=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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