

## Chemical Safety Data Sheet MSDS / SDS

## 2,4,6-tris(dimethylaminomethyl)phenol 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: 2,4,6-tris(dimethylaminomethyl)phenol

CAS: 90-72-2

**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  
Skin irritation, Category 2

Eye irritation, Category 2

**GHS label elements, including precautionary statements**

Pictogram(s)



Signal word

Warning

**Hazard statement(s)**

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

**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/...

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

**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 which do not result in classification

no data available

### SECTION 3: Composition/information on ingredients

#### Substance

Chemical name:	2,4,6-tris(dimethylaminomethyl)phenol
Common names and synonyms:	2,4,6-tris(dimethylaminomethyl)phenol
CAS number:	90-72-2
EC number:	202-013-9
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**

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. Phenols and related compounds

### **SECTION 5: Firefighting measures**

#### **Suitable extinguishing media**

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Special protective equipment for firefighters: Wear self contained breathing apparatus for fire fighting if necessary.

#### **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**

Accidental Release Measures. Personal precautions: Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Environmental precautions: Do not let product enter drains. Methods and materials for containment and cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

## **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**

Storage temperature: 2-8 deg C

## **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.
Colour:	Pale yellow/straw.
Odour:	no data available
Melting point/freezing point:	< -20.15°C. Remarks:+/- 0.5 degrees K.
Boiling point or initial boiling point and boiling range:	Ca. 594. Atm. press.:Ca. 101.325 kPa. Remarks:Decomposed from approximately 429 ± - 272.65°C at 100.72 kPa.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	149 °C.

Auto-ignition temperature:	382 °C. Remarks:382 ± 5°C.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 200. Temperature:77.0°F. Remarks:Viscosity @ 77 ° F (25 °C) (cP) = 200.
Solubility:	In water, 1.64X10+5 mg/L at 25 deg C (est)
Partition coefficient n-octanol/water:	Pow = >= 0.219. Temperature:21.5 °C. Remarks:The partition coefficient of the test material was determined to be 0.219 at 21.5 ± 1.0°C, log10 Pow -0.660.
Vapour pressure:	>= 7.5 Pa. Temperature:>= 25 °C. Remarks:The test material has been determined to have a vapor pressure of 7.5 x 10-2 Pa at 25 degrees C, using a vapor pressure balance.
Density and/or relative density:	8.1 lb/gal. Temperature:77 °F.
Relative vapour density:	>1 (vs air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Moderately soluble in water.

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

Not flammable or combustible. Amines are chemical bases. They neutralize acids to form salts plus water. These acid-base reactions are exothermic. The amount of heat that is evolved per mole of amine in a neutralization is largely independent of the strength of the amine as a base. Amines may be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides,

anhydrides, and acid halides. Flammable gaseous hydrogen is generated by amines in combination with strong reducing agents, such as hydrides. TOXICITY - Variable. Some are very poisonous; others are only slightly toxic. Many amines are skin irritants, and some are sensitizers.

**Conditions to avoid**

no data available

**Incompatible materials**

Strong oxidizing agents, Strong acids

**Hazardous decomposition products**

When heated to decomposition it emits toxic fumes of NO<sub>x</sub>.

**SECTION 11: Toxicological information**

**Acute toxicity**

Oral: LD50 Rat oral 1200 mg/kg

Inhalation: no data available

Dermal: LD50 - rat (male) - > 1 mL/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**

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 - *Cyprinus carpio* - 175 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: LC50 - *Palaemonetes vulgaris* - 718 mg/L - 96 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 84 mg/L - 72 h.

Toxicity to microorganisms: NOEC - activated sludge, domestic - 2 mg/L - 28 d. Remarks: Respiration rate.

**Persistence and degradability**

no data available

**Bioaccumulative potential**

An estimated BCF of 3 was calculated in fish for 2,4,6-tris(dimethylaminomethyl)phenol(SRC), using an estimated log Kow of 0.77(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for

bioconcentration in aquatic organisms is low(SRC).

### **Mobility in soil**

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 2,4,6-tris(dimethylaminomethyl)phenol can be estimated to be 1480(SRC). According to a classification scheme(2), this estimated Koc value suggests that 2,4,6-tris(dimethylaminomethyl)phenol is expected to have low mobility in soil. The estimated pKa's of 2,4,6-tris(dimethylaminomethyl)phenol are estimated as 8.41, 9.12 and 9.75 for the three amine groups and 10.4 for the hydroxyl group(3), indicating that this compound will exist almost entirely in cation form in the environment and cations generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4).

### **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: 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)**

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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