

## Chemical Safety Data Sheet MSDS / SDS

## Pentachlorobenzenethiol SDS

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

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

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

Product name: Pentachlorobenzenethiol

CAS: 133-49-3

**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

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

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

Eye irritation, Category 2

## GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H319 Causes serious eye irritation

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

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

Response

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

none

Other hazards which do not result in classification

no data available

## SECTION 3: Composition/information on ingredients

Substance

Chemical name: Pentachlorobenzenethiol

Common names and synonyms: Pentachlorobenzenethiol

CAS number: 133-49-3  
EC number: 205-107-8  
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

no data available

#### 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. Pentachlorophenol and Related Compounds

## SECTION 5: Firefighting measures

**Suitable extinguishing media**

Wear self contained breathing apparatus for fire fighting if necessary.

**Specific hazards arising from the chemical**

no data available

**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, protective equipment and emergency procedures Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust. For personal protection see section Environmental precautions Do not let product enter drains. Methods and materials for containment and cleaning up Pick up and arrange disposal without creating dust. Sweep up and shovel. 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**

Keep container tightly closed in a dry and well-ventilated place.

## **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:	DryPowder
Colour:	Grey solid
Odour:	no data available
Melting point/freezing point:	140°C(lit.)
Boiling point or initial boiling point and boiling range:	117°C/20mmHg(lit.)
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	98°C(lit.)
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water, 4.8X10 <sup>-3</sup> mg/L at 25 deg C (est)
Partition coefficient n-octanol/water:	log Kow = 5.91 (est)
Vapour pressure:	8.41E-05mmHg at 25°C
Density and/or relative density:	1.745 g/cm <sup>3</sup>
Relative vapour density:	no data available

Particle characteristics:

no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

Strong oxidizing agents

### Hazardous decomposition products

Carbon oxides, Sulphur oxides, Hydrogen chloride gas

## SECTION 11: Toxicological information

### Acute toxicity

Oral: LD50 Rat oral 11,900 mg/kg

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: LC100; Species: Brachydanio rerio (Zebrafish); Conditions: static bioassay; Concentration 2.8 mg/L for 96 hours



Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

#### **Persistence and degradability**

AEROBIC: Pentachlorothiophenol biodegradation of 0% was reported using a domestic sewage inoculum and a 30-day incubation period(1). Biotransformation of pentachloronitrobenzene by four soil micromycetes yielded six metabolites including pentachlorothiophenol(2).

#### **Bioaccumulative potential**

An estimated BCF of 3,700 was calculated in fish for pentachlorothiophenol(SRC), using an estimated log Kow of 5.91(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is very high, provided the compound is not metabolized by the organism(SRC).

#### **Mobility in soil**

Using a structure estimation method based on molecular connectivity indices(1), the Koc of pentachlorothiophenol can be estimated to be 6,200(SRC). According to a classification scheme(2), this estimated Koc value suggests that pentachlorothiophenol is expected to be immobile 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: UN3399 (For reference only, please check.)

IMDG: UN3399 (For reference only, please check.)

IATA: UN3399 (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER- REACTIVE, FLAMMABLE (For reference only, please check.)

IMDG: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER- REACTIVE, FLAMMABLE (For reference only, please check.)

IATA: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER- REACTIVE, FLAMMABLE (For reference only, please check.)

### Transport hazard class(es)

ADR/RID: 4.3 (For reference only, please check.)

IMDG: 4.3 (For reference only, please check.)

IATA: 4.3 (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: 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**

Not 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/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any