

# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

## SECTION 1: Identification

### 1.1 GHS Product identifier

**Product name** Pentachlorobenzenethiol

### 1.2 Other means of identification

**Product number**

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**Other names**

Benzenethiol, pentachloro-; 2,3,4,5,6-pentachlorobenzenethiol;  
Pentachlorobenzenethiol

### 1.3 Recommended use of the chemical and restrictions on use

**Identified uses**

Industrial and scientific research use.

**Uses advised against**

no data available

### 1.4 Supplier's details

**Company**

Shanghai Baishun Biotechnology Co., Ltd

**Address**

No. 26, Lane 918, Lianye Road, Zhelin Town, Fengxian  
District, Shanghai, 201400, China

**Telephone**

+86-21-37581181

### 1.5 Emergency phone number

**Emergency phone  
number**

+86-21-37581181

**Service hours**

Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT  
+8 hours).

## SECTION 2: Hazard identification

### 2.1 Classification of the substance or mixture

Eye irritation, Category 2

### 2.2 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.

<b>Response</b>	P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/... P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
<b>Storage</b>	none
<b>Disposal</b>	none

## 2.3 Other hazards which do not result in classification

no data available

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Pentachlorobenzenethiol	Pentachlorobenzenethiol	133-49-3	205-107-8	100%

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## SECTION 4: First-aid measures

### 4.1 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.

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

no data available

### 4.3 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

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## SECTION 5: Fire-fighting measures

### 5.1 Suitable extinguishing media

Wear self contained breathing apparatus for fire fighting if necessary.

### 5.2 Specific hazards arising from the chemical

no data available

### 5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

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## SECTION 6: Accidental release measures

### 6.1 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.

### 6.2 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.

### 6.3 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.

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## SECTION 7: Handling and storage

### 7.1 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.

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

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

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

### 8.2 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.

### 8.3 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

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

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

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## **SECTION 10: Stability and reactivity**

### **10.1 Reactivity**

no data available

### **10.2 Chemical stability**

Stable under recommended storage conditions.

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

no data available

### **10.4 Conditions to avoid**

no data available

### **10.5 Incompatible materials**

Strong oxidizing agents

### **10.6 Hazardous decomposition products**

Carbon oxides, Sulphur oxides, Hydrogen chloride gas

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## **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

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## **SECTION 12: Ecological information**

### **12.1 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

### **12.2 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).

### **12.3 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).

### **12.4 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.

### **12.5 Other adverse effects**

no data available

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## SECTION 13: Disposal considerations

### 13.1 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

### 14.1 UN Number

ADR/RID: UN3399 (For reference only, please check.)

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

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

### 14.2 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.)

### 14.3 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.)

### 14.4 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.)

### 14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

### 14.6 Special precautions for user

no data available

### 14.7 Transport in bulk according to IMO instruments

no data available

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## SECTION 15: Regulatory information

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

Chemical name	Common names and synonyms	CAS number	EC number
Pentachlorobenzenethiol	Pentachlorobenzenethiol	133-49-3	205-107-8
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.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Listed.
Vietnam National Chemical Inventory	Not Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Listed.
Korea Existing Chemicals List (KECL)	Listed.

## SECTION 16: Other information

### Information on revision

**Creation Date** July 15, 2019

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### 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/>

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisys.com](mailto:sds@xixisys.com)**

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