

## Chemical Safety Data Sheet MSDS / SDS

## Hexachlorocyclopentadiene 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: Hexachlorocyclopentadiene

CAS: 77-47-4

**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

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

Acute toxicity - Category 4, Oral

Acute toxicity - Category 3, Dermal

Skin corrosion, Sub-category 1B  
Acute toxicity - Category 2, Inhalation  
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

### Hazard statement(s)

H302 Harmful if swallowed  
H311 Toxic in contact with skin  
H314 Causes severe skin burns and eye damage  
H330 Fatal if inhaled  
H410 Very 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.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P271 Use only outdoors or in a well-ventilated area.  
P284 [In case of inadequate ventilation] wear respiratory protection.  
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.  
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
P363 Wash contaminated clothing before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P320 Specific treatment is urgent (see ... on this label).  
P391 Collect spillage.

#### **Storage**

P405 Store locked up.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

#### **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:	Hexachlorocyclopentadiene
Common names and synonyms:	Hexachlorocyclopentadiene
CAS number:	77-47-4
EC number:	201-029-3
Concentration:	100%

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

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

#### **If inhaled**

Fresh air, rest. Half-upright position. Artificial respiration may be needed. Refer for medical attention.

### **Following skin contact**

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

### **Following eye contact**

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

### **Following ingestion**

Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink. Refer for medical attention .

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

This compound is very toxic and may be fatal if inhaled, swallowed, or absorbed through the skin. The probable human lethal dose is 50-500 mg/kg, or between 1 teaspoon and 1 ounce for a 150 lb. (70 kg) person. Severe exposure induces pulmonary hyperemia and edema, degenerative and necrotic changes in brain, heart and adrenal glands and necrosis of liver and kidney tubules. (EPA, 1998)

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

#### **Absorption, Distribution and Excretion**

Rats given 6 mg/kg hexachlorocyclopentadiene (HEX) orally excreted 33% in urine, 10% in feces in 7 days. Most excretion occurred during 1st 24 hr after dosing. Kidney retained 0.5%, liver >0.5%. Biliary excretion of only 16% with 66% still voided in the feces of bile duct cannulated rats suggested that the majority of orally consumed HEX was not absorbed. Degradation apparently occurred in the gut since little of the fecal material was of an apolar nature. The kidney, liver, ovaries and fat were the major sites of deposition of (14)C-HEX equivalents. In rats, the kidney contained the highest levels of residues, whereas in mice the residues in the liver exceeded those in the kidney. Other than this difference, the fate of HEX in rats and mice, both male and female, was quite similar and in each case the tissue residues reached a plateau after about two weeks on the HEX-containing diets. [Mehendale HM; Environ Health Perspect 21: 275-78 (1977)] Full text: PMC1475343

## **SECTION 5: Firefighting measures**

### **Suitable extinguishing media**

If material involved in fire: Extinguish fire using agent suitable for type of surrounding fire (material itself does not burn or burns with difficulty). Use water spray to knock-down vapors.

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

Toxic hydrogen chloride, chlorine, and phosgene gases may form in fires. In presence of moisture, will corrode iron and other

materials; flammable and explosive hydrogen gas may collect in enclosed space. Will corrode iron and other metals in the presence of moisture. Reacts slowly with water to form hydrochloric acid; however, the reaction is not hazardous. Hazardous polymerization may not occur. (EPA, 1998)

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

In case of fire in the surroundings, use appropriate extinguishing media.

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

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

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable plastic containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

#### **Environmental precautions**

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable plastic containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

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

Environmental considerations. Land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner. / Cover solids with a plastic sheet to prevent dissolving in rain or fire fighting water. Absorb bulk liquid with fly ash or cement powder.

### **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 in an area without drain or sewer access. Dry. Well closed. Ventilation along the floor.

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

TLV: 0.01 ppm as TWA; A4 (not classifiable as a human carcinogen).MAK skin absorption (H)

### 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 face shield or eye protection in combination with breathing protection.

#### Skin protection

Protective gloves. Protective clothing.

#### Respiratory protection

Use ventilation, local exhaust or breathing protection.

#### Thermal hazards

no data available

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

**Physical state:** Hexachlorocyclopentadiene is a pale yellow liquid with a pungent odor. Density 14.3 lb /gal. Solidifies at 50°F. Insoluble in water. Noncombustible. Very toxic by skin absorption and inhalation. Corrosive to tissue.

**Colour:** Dense, oily liquid

Odour:	Pungent, unpleasant odor.
Melting point/freezing point:	-10°C
Boiling point or initial boiling point and boiling range:	239°C
Flammability:	Noncombustible Liquid
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	150°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	less than 0.1 mg/mL at 70.7° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Kow= 5.04
Vapour pressure:	0.13 psi ( 20 °C)
Density and/or relative density:	1.702
Relative vapour density:	9.4 (EPA, 1998) (Relative to Air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Decomposes on heating. This produces toxic and corrosive fumes including hydrogen chloride and phosgene. Reacts with moist air. This produces hydrogen chloride (see ICSC 0163). Attacks many metals in the presence of water. This produces flammable/explosive gas (hydrogen - see ICSC 0001).

### Chemical stability

no data available

### Possibility of hazardous reactions

NonflammableThe vapour is heavier than air.HEXACHLOROCYCLOPENTADIENE is incompatible with strong oxidizing and reducing agents. Also incompatible with many amines, nitrides, azo/diazo compounds, alkali metals (sodium), and epoxides.

### Conditions to avoid

no data available

### Incompatible materials

Reacts slowly with water to form hydrochloric acid.

### Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /hydrogen chloride/.

## SECTION 11: Toxicological information

### Acute toxicity

Oral: LD50 Albino Rat oral 300-630 mg/kg

Inhalation: LC50 Rat (Sprague-Dawley, young adult male) inhalation 18.1 mg/cu m/4 hr

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**

Cancer Classification: Group D Not Classifiable as to Human Carcinogenicity

#### **Reproductive toxicity**

No information is available regarding the reproductive or developmental effects of hexachlorocyclopentadiene in humans. Animal studies have not reported birth defects from exposure to hexachlorocyclopentadiene by gavage (placing the chemical experimentally in the stomach), and no information is available regarding reproductive or developmental effects from inhalation exposure. (-)

#### **STOT-single exposure**

The substance is corrosive to the eyes, skin and respiratory tract. Corrosive on ingestion. Inhalation may cause lung oedema. See Notes. The substance may cause effects on the kidneys and liver. This may result in tissue lesions. The effects may be delayed. Medical observation is indicated.

#### **STOT-repeated exposure**

no data available

#### **Aspiration hazard**

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C.

## SECTION 12: Ecological information

### Toxicity

Toxicity to fish: LC50 Pimephales promelas (Fathead minnow, early juvenile) 6.7 ug/L/30 days; flow-through

Toxicity to daphnia and other aquatic invertebrates: LC50 Daphnia magna 93 ug/L/24 hr (95% confidence interval: 78.9-109.6 ug/L); 52 ug/L/48 hr (95% confidence interval: 44.8-60.9 ug/L); static, 17 deg C, soft water /from table

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

### Persistence and degradability

In a static-screening study (BOD dilution water containing nutrient broth, settled domestic wastewater as inoculum, initial hexachlorocyclopentadiene concn 5 and 10 mg/l, during a 7 day incubation period in the dark) 100% loss of hexachlorocyclopentadiene was observed(1). Based on hydrolytic half-life data for this compound, hydrolysis alone does not necessarily account for the 100% observed loss of hexachlorocyclopentadiene. Volatilization was reported to be insignificant. Thus, some of the observed loss may have been due to biodegradation(SRC). Hexachlorocyclopentadiene has been found to degrade more quickly in nonsterile soils than sterile soils, suggesting that degradation was partially due to biodegradation(2).

### Bioaccumulative potential

Bioconcentration factor of hexachlorocyclopentadiene in a laboratory model ecosystem were: alga (Edogonium) 341; snail (Physa) 929; mosquito (Culex) 1634; and fish (Gambusia) 448(1). BCFs in other aquatic species were: green alga (Chlorella fusca) 1090(2); fathead minnow (Pimephales promelas) <11(3) and 29(4); goldfish (Carassius auratus) 100-323(5), golden orfe (Leuciscus idus) 1230(6). The steady-state BCF value for fingerling goldfish exposed to 4 and 5 ppb of hexachlorocyclopentadiene was 1354 in a renewable freshwater system, and the BCF was 323 in a static system(7). Based on a classification scheme(8), these data indicate that bioconcentration in aquatic organisms is very high(SRC).

### Mobility in soil

The attenuation mechanisms & capacity of selected clay minerals and soils for hexachlorocyclopentadiene (C-56) adsorption, a chemical model to predict C-56 migration through soil materials, & the major degradation products of C-56 in the environment were investigated. C-56 was readily adsorbed by soil materials; the adsorption capacity of C-56 was highly correlated with the total organic carbon content. Adsorbed C-56 remained immobile in the earth materials when leached with water, landfill leachates, and caustic soda brine solutions, but was highly mobile when leached with organic solvents.

### 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: UN2646 (For reference only, please check.)

IMDG: UN2646 (For reference only, please check.)

IATA: UN2646 (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: HEXACHLOROCYCLO- PENTADIENE (For reference only, please check.)

IMDG: HEXACHLOROCYCLO- PENTADIENE (For reference only, please check.)

IATA: HEXACHLOROCYCLO- PENTADIENE (For reference only, please check.)

### 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**

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/>

### **Other Information**

The symptoms of lung oedema often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation is therefore essential. Immediate administration of an appropriate inhalation therapy by a doctor or a person authorized by him/her, should be considered.

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