Chemical Book India

Chemical Safety Data Sheet MSDS / SDS

Hexachlorobuta-1,3-diene 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: Hexachlorobuta-1,3-diene

CAS: 87-68-3

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

Relevant identified For R&D use only. Not for medicinal, household or other use.

uses:

Uses advised none

against:

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 4, Dermal Skin irritation, Category 2
Skin sensitization, Category 1
Acute toxicity - Category 4, Inhalation
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word Warning

Hazard statement(s)

H302 Harmful if swallowed

H312 Harmful in contact with skin

H315 Causes skin irritation

H317 May cause an allergic skin reaction

H332 Harmful if inhaled

H400 Very toxic to aquatic life

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/...

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

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

P271 Use only outdoors or in a well-ventilated area.

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/...

P317 Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P332+P317 If skin irritation occurs: Get medical help.

P333+P317 If skin irritation or rash occurs: Get medical help.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P391 Collect spillage.

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: Hexachlorobuta-1,3-diene
Common names and Hexachlorobuta-1,3-diene

synonyms:

CAS number: 87-68-3
EC number: 201-765-5
Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. 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

Poisonous; may be fatal if inhaled, swallowed or absorbed through the skin. Inhalation causes repiratory difficulty and irritation of mucous membranes. Skin and eye irritant; may cause burns. (USCG, 1999)

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

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 . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Cover skin burns with sterile dressings after decontamination . Halogenated aliphatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

To fight fire, use dry chemical, CO2, alcohol foam, water spray, fog, mist.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: They contain highly toxic and irritating chloride fumes. Behavior in Fire: May burn to produce highly toxic and irritating gases. (USCG, 1999)

Special protective actions for fire-fighters

Use water spray, powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: complete protective clothing including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable 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: complete protective clothing including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable 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

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.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. 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

Separated from food and feedstuffs. Well closed. Ventilation along the floor. Store in an area without drain or sewer access. Provision to contain effluent from fire extinguishing.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.02 ppm as TWA; (skin); A3 (confirmed animal carcinogen with unknown relevance to humans). MAK: 0.22 mg/m3, 0.02 ppm; peak limitation category: II(2); skin absorption (H); carcinogen category: 4; pregnancy risk group: C

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: Hexachlorobutadiene is a colorless liquid with a mild odor. Insoluble in water and denser

than water. Nonflammable. May be toxic by ingestion or inhalation. Used as a solvent and

heat transfer fluid.

Colour: Clear, colorless liquid

Odour: Mild, turpentine-like odor.

Melting -19°C

point/freezing

point:

Boiling point or 210-220°C(lit.)

initial boiling point and boiling range:

Flammability: Combustible Liquid

Lower and upper

no data available

explosion

limit/flammability

limit:

Flash point: 92.2°C

Auto-ignition

1130° F (USCG, 1999)

temperature:

Decomposition r

no data available

temperature:

pH: no data available

Kinematic 2.447 centipoise at 37.7 deg C, 1.479 centistokes; 1.131 centipoise at 98.8 deg C, 0.724

viscosity: centistokes.

Solubility: less than 0.1 mg/mL at 72° F (NTP, 1992)

Partition log Kow = 4.78

coefficient noctanol/water:

Vapour pressure: 0.2 mm Hg (20 °C)

Density and/or 1.655

relative density:

Relative vapour 8.99 (NTP, 1992) (Relative to Air)

density:

Particle no data available

characteristics:

SECTION 10: Stability and reactivity

Reactivity

NIOSH considers hexachlorobutadiene to be a potential occupational carcinogen.

Decomposes on burning. This produces toxic and corrosive fumes including hydrogen chloride (see ICSC 0163) and phosgene (see ICSC 0007). Attacks rubber and some forms of plastic.

Chemical stability

no data available

Possibility of hazardous reactions

Combustible when exposed to heat or flame; can react vigorously with oxidizing materials. HEXACHLOROBUTADIENE rapidly decomposes rubber on contact. Can react vigorously with oxidizing materials. Reacts to form an explosive product with bromine perchlorate. (NTP, 1992). Gives highly toxic and irritating chloride fumes when burned.

Conditions to avoid

no data available

Incompatible materials

Oxidizers.

Hazardous decomposition products

When heated to decomposition it emits very toxic fumes of /chlorine/ Cl-.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Guinea pig single oral 90 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

EPA: Possibly carcinogenic to humans. IARC: Not classifiable as to carcinogenicity to humans. NTP: Not evaluated

Reproductive toxicity

No information is available regarding the developmental or reproductive effects of hexachlorobutadiene in humans. One study reported that the frequency of abnormal sperm morphology did not increase significantly over controls in mice exposed to hexachlorobutadiene via inhalation. A study in rats exposed via inhalation reported no embryotoxic effects, except for a reduction in fetal body weights. Oral animal studies have reported reduced fertility, reduced fetal body weights, but no birth defects or other developmental effects from hexachlorobutadiene exposure.

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. The liquid is corrosive. The substance may cause effects on the kidneys.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization. May cause genetic damage in humans.

Aspiration hazard

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

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

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: Hexachloro-1,3-butadiene may biodegrade in natural waters since 100% degradation occurred in 7 days in an aerobic batch culture incubated at 25 deg C and inoculated with settled domestic sewage(1). Estimated half-lives for hexachloro-1,3-butadiene disappearance based on monitoring data are 3-30 days in river water and 30-300 days in lake and ground waters(2). ANAEROBIC: Greater than 99% of hexachloro-1,3-butadiene transformed to (E,E)-1,2,3,4-tetrachlorobutadiene by reductive dechlorination in columns with Rhine sediment (Germany) operated at 20 deg C with methanogenic electron acceptors(3). Hexachloro-1,3-butadiene was only removed under methanogenic conditions using these sediments and not when oxygen or nitrate were present in the column experiments(4). Reductive dechlorination in the column was ascribed to the activity of anaerobic microorganisms(4).

Bioaccumulative potential

The mean bioconcentration factor (BCF) for rainbow trout exposed to 0.10 ng/l and 3.4 ng/l of hexachloro-1,3-butadiene was 5,800 and 17,000, respectively(1). The BCF for fathead minnow exposed to hexachloro-1,3-butadiene was 6,918(2). According to a classification scheme(3), these BCF values suggest bioconcentration in aquatic organisms is very high. The mean bioconcentration factor for hexachloro-1,3-butadiene between oligocheate worms and sediment in Lake Ontario near the Niagara River was 0.43(4). The concn of the chemical in the sediment pore water was the main factor affecting bioconcentration(4).

Mobility in soil

The Koc of hexachloro-1,3-butadiene ranges from 5.02X10+3 to 2.75X10+5(1-3). According to a classification scheme(4), these Koc values suggest that hexachloro-1,3-butadiene has slight to no mobility in soil(SRC).

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: UN2279 (For reference only, please check.) IMDG: UN2279 (For reference only, please check.) IATA: UN2279 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: HEXACHLOROBUTADIENE (For reference only, please check.) IMDG: HEXACHLOROBUTADIENE (For reference only, please check.) IATA: HEXACHLOROBUTADIENE (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: III (For reference only, please check.)
IMDG: III (For reference only, please check.)
IATA: III (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)

Not 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

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-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

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