

Chemical Safety Data Sheet MSDS / SDS

4-vinylcyclohexene 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: 4-vinylcyclohexene
CAS: 100-40-3

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

Relevant identified uses: For R&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**

Carcinogenicity, Category 2

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H351 Suspected of causing cancer

Precautionary statement(s)

Prevention

P203 Obtain, read and follow all safety instructions before use.

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

Response

P318 IF exposed or concerned, get medical advice.

Storage

P405 Store locked up.

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: 4-vinylcyclohexene

Common names and synonyms: 4-vinylcyclohexene

CAS number: 100-40-3
EC number: 202-848-9
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

Remove contaminated clothes. Rinse skin with plenty of water or shower.

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

Refer for medical attention .

Most important symptoms/effects, acute and delayed

Exposure can cause irritation of eyes, nose and throat. High concentrations have a narcotic effect. (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 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 . Aliphatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

To fight fire, use foam, CO₂, dry chemical.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: Irritating vapors and toxic gases, such as carbon dioxide and carbon monoxide, may be formed when involved in fire. Behavior in Fire: Vapors can flow along surfaces to distant ignition source and flash back. (USCG, 1999)

Special protective actions for fire-fighters

Use foam, powder, 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: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in dry sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in dry sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer.

Methods and materials for containment and cleaning up

PRECAUTIONS FOR "CARCINOGENS": A high-efficiency particulate arrestor (HEPA) or charcoal filters can be used to minimize amt of carcinogen in exhausted air ventilated safety cabinets, lab hoods, glove boxes or animal rooms ... Filter housing that is designed so that used filters can be transferred into plastic bag without contaminating maintenance staff is avail commercially. Filters should be placed in plastic bags immediately after removal ... The plastic bag should be sealed immediately ... The sealed bag should be labelled properly ... Waste liquids ... should be placed or collected in proper containers for disposal. The lid should be secured & the bottles properly labelled. Once filled, bottles should be placed in plastic bag, so that outer surface ... is not contaminated ... The plastic bag should also be sealed & labelled. ... Broken glassware ... should be decontaminated by solvent extraction, by chemical destruction, or in specially designed incinerators. Chemical Carcinogens

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. NO contact with oxidizing agents. Closed system, ventilation, explosion-proof electrical equipment and lighting. Do NOT use compressed air for filling, discharging, or 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

Fireproof. Separated from oxidants. Cool. Store only if stabilized. PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemophysical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. Chemical Carcinogens

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.1 ppm as TWA; A3 (confirmed animal carcinogen with unknown relevance to humans). MAK: skin absorption (H); carcinogen category: 2

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 safety goggles 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:	Liquid.
Colour:	Colourless.
Odour:	no data available
Melting point/freezing point:	-108.7 °C. Atm. press.:Ca. 1 013 hPa. Remarks:Pressure not reported. Atmospheric pressure can be assumed.
Boiling point or initial boiling point and boiling range:	129 °C. Atm. press.:Ca. 1 013 hPa. Remarks:Pressure not reported. Atmospheric pressure can be assumed.
Flammability:	Highly flammable.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	14 °C. Atm. press.:Ca. 1 013 hPa.
Auto-ignition temperature:	280 °C. Atm. press.:Ca. 1 013 hPa. Remarks:The pressure has not been reported. Atmospheric pressure can be assumed.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 0.69. Temperature:20°C.;kinematic viscosity (in mm ² /s) = 0.83. Temperature:20°C.

Solubility:	1 to 10 mg/mL at 67.1° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = 3.93. Remarks:PH and temperature not reported. pH not relevant.
Vapour pressure:	15 hPa. Temperature:20 °C.
Density and/or relative density:	0.83 g/cm ³ . Temperature:20 °C.
Relative vapour density:	3.76 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance can form explosive peroxides. Reacts with oxidants. This generates fire and explosion hazard.

Chemical stability

Oxidizes in air to form hydroperoxide

Possibility of hazardous reactions

FLAMMABLE, DANGEROUS FIRE RISK. The vapour mixes well with air, explosive mixtures are easily formed. VINYL CYCLOHEXENE can react with oxidizing materials. It is also incompatible with peroxide catalysts. Prolonged exposure to oxygen-containing gases leads to discoloration and gum formation. (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

Can react with oxidizers.

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 6 300 mg/kg bw.

Inhalation: LC50 - rat - 6 095 ppm.

Dermal: LD50 - rabbit - 20 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

Evaluation: There is inadequate evidence in humans for the carcinogenicity of 4-vinyl-1-cyclohexene. There is sufficient evidence in experimental animals for the carcinogenicity of 4-vinyl-1-cyclohexene. Overall evaluation: 4-Vinyl-1-cyclohexene is possibly carcinogenic to humans (Group 2B).

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes and skin.

STOT-repeated exposure

This substance is possibly carcinogenic to humans.

Aspiration hazard

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

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oryzias latipes* - 17 mg/L - 48 h.

Toxicity to daphnia and other aquatic invertebrates: EC 10 / 50 /100 - *Daphnia magna* - > 200 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 6.15 mg/L - 72 h.

Toxicity to microorganisms: EC50 - sewage, domestic - > 200 mg/L - 16 h.

Persistence and degradability

AEROBIC: 4-Vinylcyclohexene, present at 100 mg/l, reached 0% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/l and the modified Japanese MITI test(1). Therefore, this compound is not expected to biodegrade rapidly in the environment(SRC).

Bioaccumulative potential

An estimated BCF of 571 was calculated for 4-vinylcyclohexene(SRC), using a log Kow of 3.93(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC).

Mobility in soil

The Koc of 4-vinylcyclohexene is estimated as 3300(SRC), using a measured log Kow of 3.93(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 4-vinylcyclohexene is expected to have slight 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: UN3295 (For reference only, please check.)

IMDG: UN3295 (For reference only, please check.)

IATA: UN3295 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

IMDG: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

IATA: HYDROCARBONS, LIQUID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 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

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

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

Do NOT take working clothes home. An added stabilizer or inhibitor can influence the toxicological properties of this substance, consult an expert. Check for peroxides prior to distillation; eliminate if found.

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