Chemical Safety Data Sheet MSDS / SDS

Cyclododeca-1,5,9-triene SDS

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

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

Product identifier

Product name: Cyclododeca-1,5,9-triene

CAS: 4904-61-4

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

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SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 3
Aspiration hazard, Category 1

Skin irritation, Category 2
Carcinogenicity, Category 2
Reproductive toxicity, Category 2
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)

H226 Flammable liquid and vapour
H304 May be fatal if swallowed and enters airways
H315 Causes skin irritation
H351 Suspected of causing cancer
H361 Suspected of damaging fertility or the unborn child
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P203 Obtain, read and follow all safety instructions before use.
P273 Avoid release to the environment.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P331 Do NOT induce vomiting.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P321 Specific treatment (see ... on this label).
P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P318 IF exposed or concerned, get medical advice.
P391 Collect spillage.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.
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:	Cyclododeca-1,5,9-triene
Common names and synonyms:	Cyclododeca-1,5,9-triene
CAS number:	4904-61-4
EC number:	225-533-8
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

Exposure can cause irritation and burns of eyes, nose and throat. (USCG, 1999)

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 if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the 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. Aliphatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Extinguish fire using agent suitable for type of surrounding fire (Material itself does not burn or burns with difficulty.) Keep run-off water out of sewers and water sources.

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

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

SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a POTW is acceptable only after review by the governing authority. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must meet Hazardous Material Criteria 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

All isomers of cyclododecatriene and their hydrogenation products are preferably stored in tanks and transported in pipelines or stainless steel or aluminum containers as a liquid. If the all-trans product is a major isomer, tanks, pipelines and containers must be heated slightly. Generally, the unsaturated compounds are covered with an inert gas to avoid oxidation reactions, and should contain an inhibitor unless they are to be processed immediately.

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:	1,5,9-cyclododecatriene is a colorless liquid. Toxic by skin absorption and ingestion and irritating to skin and eyes. Used to make other chemicals.

Colour:	Colorless
Odour:	Terpene-like odor
Melting point/freezing point:	33-35°C(lit.)
Boiling point or initial boiling point and boiling range:	240°C at 760 mmHg
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	87.8°C
Auto-ignition temperature:	244 deg C
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water, 0.47 mg/L at 25 deg C (est)
Partition coefficient n-octanol/water:	log Kow = 5.50
Vapour pressure:	0.07 mm Hg at 25 deg C (est)
Density and/or relative density:	0.89 g/mL at 20°C(lit.)
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

No rapid reaction with air. No rapid reaction with water.

Chemical stability

no data available

Possibility of hazardous reactions

1,5,9-CYCLODODECATRIENE may react vigorously with strong oxidizing agents. May react exothermically with reducing agents to release hydrogen gas. In the presence of various catalysts (such as acids) or initiators, may undergo exothermic addition polymerization reactions.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat oral 1780-2300 mg/kg

Inhalation: LC50 Rat inhalation 7.5-8.9 mg/L for 6 hours

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: LC50; Species: Oncorhynchus mykiss (Rainbow trout); Conditions: static bioassay; Concentration: 5.5 mg/L for 96 hours

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: EC50; Species: Selenastrum capricornutum (Algae); Conditions: static bioassay; Concentration: 140 mg/L for 4 days; Effect: decrease in growth rate

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: 1,5,9-Cyclododecatriene, present at 100 mg/L, reached 0% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(1). 1,5,9-Cyclododecatriene reached 1% of the theoretical oxygen demand in a 5 day BOD test(2,3).

Bioaccumulative potential

1,5,9-Cyclododecatriene's production and use as a feedstock, for the manufacturing of C12-polyamides, dodecanoic acid, and in flame retardants(1) may result in its release to the environment through various waste streams(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 1,5,9-cyclododecatriene can be estimated to be 5300(SRC). According to a classification scheme(2), this estimated Koc value suggests that 1,5,9-cyclododecatriene 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: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (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

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

(PICCS)

Not 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/