

Chemical Safety Data Sheet MSDS / SDS

3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate 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: 3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate

CAS: 4098-71-9

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**

Skin irritation, Category 2

Eye irritation, Category 2

Skin sensitization, Category 1
Acute toxicity - Category 3, Inhalation
Specific target organ toxicity - single exposure, Category 3
Respiratory sensitization, Category 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H315 Causes skin irritation
H319 Causes serious eye irritation
H317 May cause an allergic skin reaction
H331 Toxic if inhaled
H335 May cause respiratory irritation
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled
H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
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.
P284 [In case of inadequate ventilation] wear respiratory protection.
P273 Avoid release to the environment.

Response

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.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continue rinsing.
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.
P316 Get emergency medical help immediately.
P319 Get medical help if you feel unwell.
P342+P316 If experiencing respiratory symptoms: Get emergency medical help immediately.
P391 Collect spillage.

Storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed.
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:	3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate
Common names and synonyms:	3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate
CAS number:	4098-71-9
EC number:	223-861-6
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Half-upright position. Refer immediately for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .

Following eye contact

Rinse with plenty of water (remove contact lenses if easily possible). Refer immediately 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 material is highly toxic by inhalation and moderately toxic through the skin. (Non-Specific -- Isocyanates) People with skin or respiratory problems should avoid exposure. (EPA, 1998)

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. Isocyanates, aliphatic thiocyanates, and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Extinguish fire using agent suitable for type of surrounding fire. (Material itself does not burn or burns with difficulty.) Use water in flooding quantities as fog. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use foam, dry chemical, or carbon dioxide. Keep run-off water out of sewers and water sources.

Specific hazards arising from the chemical

When heated to decomposition, it emits toxic fumes of nitrogen oxides. (EPA, 1998)

Special protective actions for fire-fighters

Use water spray, foam, powder, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: chemical protection suit including self-contained breathing apparatus. Collect leaking liquid in covered containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Treat remaining liquid with a mixture of ammonia (4-8%), detergent (2%), and water. Do NOT let this chemical enter the environment.

Environmental precautions

Personal protection: chemical protection suit including self-contained breathing apparatus. Collect leaking liquid in covered containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Treat remaining liquid with a mixture of ammonia (4-8%), detergent (2%), and water. Do NOT let this chemical enter the environment.

Methods and materials for containment and cleaning up

Decontamination of spilled isocyanates and disposal of isocyanate waste are best conducted by using aqueous ammonia (3-8% concentrated ammonia solution in 90-95% water with 0.2-5% liquid detergent) or aqueous sodium carbonate (5-10% sodium carbonate in 90-95% water and 0.2-5% liquid detergent). An alcoholic solution (50% ethanol, isopropyl alcohol, or butanol; 45% water; and 5% concentrated ammonia) may be preferred because of the low miscibility of isocyanates with water. Isocyanates

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 bases, acids, alcohols, amines, amides, phenols, mercaptans and food and feedstuffs. Keep in a well-ventilated room. Well closed. Cool. Dry. Store in an area without drain or sewer access. Isocyanates are transported in railroad tank cars, tank trucks, tanks in ships, containers, and drums. They are stored in steel tanks and processed in steel equipment. For long-term storage stainless steel is recommended. To avoid contamination by atmospheric moisture, a dry air or inert gas blanket is essential. Isocyanates

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.005 ppm as TWA.MAK: 0.046 mg/m³, 0.005 ppm; peak limitation category: I(1); sensitization of respiratory tract and skin (SAH); pregnancy risk group: D

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 closed system.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Light yellowish.
Odour:	Pungent

Melting point/freezing point:	-60 °C.
Boiling point or initial boiling point and boiling range:	310 °C. Atm. press.:1 013 hPa.
Flammability:	Class IIIB Combustible Liquid: Fl.P. at or above 200°F.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	150.5 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature:	430 °C. Atm. press.:Ca. 1 013 hPa.
Decomposition temperature:	310°C
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 14.2. Temperature:20°C. Remarks:Shear rate 1000/s.;dynamic viscosity (in mPa s) = 7.41. Temperature:40°C. Remarks:Shear rate 1000/s.;dynamic viscosity (in mPa s) = >= 18 - <= 26. Temperature:20°C. Remarks:Shear rate 20/s - 100/s.
Solubility:	less than 1 mg/mL at 77° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = 0.99. Temperature:23 °C. Remarks:PH value is for test water saturated with octanol but without test substance.
Vapour pressure:	0.001 hPa. Temperature:20 °C.
Density and/or relative density:	1 058 kg/m3. Temperature:20 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance may polymerize. Decomposes on burning. This produces toxic and corrosive fumes including hydrogen cyanide and nitrogen oxides. Reacts with acids, alcohol, amines, bases, amides, phenols and mercaptans. This generates toxic, fire and explosion hazard. Attacks plastics and rubber.

Chemical stability

no data available

Possibility of hazardous reactions

A flammable liquid. ISOPHORONE DIISOCYANATE reacts with all substances containing active hydrogen atoms such as water, alcohols, phenols, amines, mercaptans, amides, urethanes and ureas. (NTP, 1992)

Conditions to avoid

no data available

Incompatible materials

Reacts with all substances containing active hydrogen atoms such as water, alcohols, phenols, amines, mercaptans, amides, urethanes, and ureas.

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /nitrogen oxides and hydrogen cyanide/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat oral greater than 1000 mg/kg

Inhalation: LC50 Rat inhalation 123 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

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is corrosive to the skin. The substance is severely irritating to the eyes. The aerosol is irritating to the respiratory tract.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization. Repeated or prolonged inhalation may cause asthma. See Notes.

Aspiration hazard

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

SECTION 12: Ecological information**Toxicity**

Toxicity to fish: LC50 - Cyprinus carpio - > 208 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 27 mg/L - 48 h. Remarks:(DOC).

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - > 70 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - 263 mg/L - 3 h. Remarks:Respiration rate.

Persistence and degradability

no data available

Bioaccumulative potential

Isocyanates, such as isophorone diisocyanate, are hydrolyzed rapidly by water(1), indicating that bioconcentration is not an important environmental fate process(SRC).

Mobility in soil

Isocyanates, such as isophorone diisocyanate, are hydrolyzed rapidly by water(1), indicating that adsorption is not an important environmental fate process(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: UN2478 (For reference only, please check.)

IMDG: UN2478 (For reference only, please check.)

IATA: UN2478 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ISOCYANATES, FLAMMABLE, TOXIC, N.O.S. or ISOCYANATE SOLUTION, FLAMMABLE, TOXIC, N.O.S. (For reference only, please check.)

IMDG: ISOCYANATES, FLAMMABLE, TOXIC, N.O.S. or ISOCYANATE SOLUTION, FLAMMABLE, TOXIC, N.O.S. (For reference only, please check.)

IATA: ISOCYANATES, FLAMMABLE, TOXIC, N.O.S. or ISOCYANATE SOLUTION, FLAMMABLE, TOXIC, 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: II (For reference only, please check.)

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

IATA: II (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

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

Anyone who has shown symptoms of asthma due to this substance should avoid all further contact. The odour warning when the exposure limit value is exceeded is insufficient. Do NOT take working clothes home.

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