

Chemical Safety Data Sheet MSDS / SDS

Isocyanatocyclohexane

Revision Date:2025-02-01 Revision Number:1

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

Product identifier

Product name : Isocyanatocyclohexane
CBnumber : CB8399629
CAS : 3173-53-3
EINECS Number : 221-639-3
Synonyms : cyclohexyl,CYCLOHEXYL ISOCYANATE

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
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 3
Acute toxicity - Category 3, Oral
Acute toxicity - Category 3, Dermal
Skin irritation, Category 2
Eye irritation, Category 2
Acute toxicity - Category 2, Inhalation
Respiratory sensitization, Category 1
Specific target organ toxicity – single exposure, Category 3

Label elements

Pictogram(s)

Signal word : Danger

Hazard statement(s)

H226 Flammable liquid and vapour

H301 Toxic if swallowed
H311 Toxic in contact with skin
H315 Causes skin irritation
H317 May cause an allergic skin reaction
H318 Causes serious eye damage
H319 Causes serious eye irritation
H330 Fatal if inhaled
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled
H335 May cause respiratory irritation
H401 Toxic to aquatic life
H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s)

P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P284 Wear respiratory protection.
P310 Immediately call a POISON CENTER or doctor/physician.
P320 Specific treatment is urgent (see ... on this label).
P330 Rinse mouth.
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position 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.
Continuerinsing.
P405 Store locked up.

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.
P270 Do not eat, drink or smoke when using this product.
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.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

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.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P316 Get emergency medical help immediately.

P361+P364 Take off immediately all contaminated clothing and wash it before reuse.

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.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P320 Specific treatment is urgent (see ... on this label).

P342+P316 If experiencing respiratory symptoms: Get emergency medical help immediately.

P319 Get medical help if you feel unwell.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: Isocyanatocyclohexane
Synonyms	: cyclohexyl,CYCLOHEXYL ISOCYANATE
CAS	: 3173-53-3
EC number	: 221-639-3
MF	: C7H11NO
MW	: 125.17

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. 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 . Wear protective gloves when administering first aid.

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

Give a slurry of activated charcoal in water to drink. Do NOT induce vomiting. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: TOXIC; inhalation, ingestion or contact (skin, eyes) with vapors, dusts or substance may cause severe injury, burns or death. Bromoacetates and chloroacetates are extremely irritating/lachrymators. Reaction with water or moist air will release toxic, corrosive or flammable gases. Reaction with water may generate much heat that will increase the concentration of fumes in the air. Fire will produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

Indication of any immediate medical attention and special treatment needed

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

Extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use "alcohol" foam, dry chemical or carbon dioxide. Keep run-off water out of sewers and water sources.

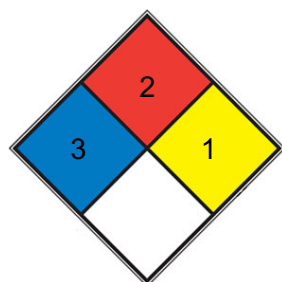
Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapors may travel to source of ignition and flash back. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Substance will react with water (some violently) releasing flammable, toxic or corrosive gases and runoff. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated or if contaminated with water. (ERG, 2016)

Advice for firefighters

Use foam, alcohol-resistant foam, powder, carbon dioxide, dry sand. In case of fire: keep drums, etc., cool by spraying with water. NO direct contact with water. Combat fire from a sheltered position.

NFPA 704



■ HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen , sulfuric acid , calcium hypochlorite , hexafluorosilicic acid)
		Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
■ FIRE	2	
■ REACT	1	Normally stable, but can become unstable at elevated temperatures and pressures (e.g. propene)
□ SPEC.		
□ HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Consult an expert! Ventilation. 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. Do NOT wash away into sewer. Personal protection: complete protective clothing including self-contained breathing apparatus.

Environmental precautions

Consult an expert! Ventilation. 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. Do NOT wash away into sewer. Personal protection: complete protective clothing including self-contained breathing apparatus.

Methods and materials for containment and cleaning up

Consult an expert! Ventilation. 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. Do not wash away into sewer. Personal protection: complete protective clothing including self-contained breathing apparatus.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 48°C use a closed system, ventilation and explosion-proof electrical equipment. Prevent build-up of electrostatic charges (e.g., by grounding). 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 strong oxidants, strong bases, strong acids and food and feedstuffs. Dry. Keep in a well-ventilated room.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Cyclohexyl isocyanate			
CAS No.	3173-53-3			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m³	ppm	mg/m³
Poland	?	0,04	?	?
	Remarks			

Biological limit values

no data available

Exposure 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

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

Information on basic physicochemical properties

Physical state	Liquid
Colour	Clear colorless to light amber
Odour	no data available
Melting point/freezing point	26°C(lit.)
Boiling point or initial boiling point and boiling range	175°C
Flammability	Flammable. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	48°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Chloroform (Sparingly)
Partition coefficient n-octanol/water	log Kow = 3.06 (est)

Vapour pressure	1.83 psi (20 °C)
Density and/or relative density	0.98
Relative vapour density	(air = 1): 4.3
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance may polymerize due to heating and under the influence of various chemicals including organometallic compounds.

Decomposes on burning. This produces toxic fumes of hydrogen cyanide and nitrogen oxides. Reacts with oxidants, strong bases, water, alcohol, acids and amines.

Chemical stability

no data available

Possibility of hazardous reactions

The vapour is heavier than air and may travel along the ground; distant ignition possible. Isocyanates and thioisocyanates are incompatible with many classes of compounds, reacting exothermically to release toxic gases. Reactions with amines, aldehydes, alcohols, alkali metals, ketones, mercaptans, strong oxidizers, hydrides, phenols, and peroxides can cause vigorous releases of heat. Acids and bases initiate polymerization reactions in these materials. Some isocyanates react with water to form amines and liberate carbon dioxide. Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence [Wischmeyer 1969].

Conditions to avoid

no data available

Incompatible materials

Reacts with oxidants, strong bases, water, alcohol, acids and amines.

Hazardous decomposition products

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

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 560 mg/kg bw
- 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

no data available

Reproductive toxicity

no data available

STOT-single exposure

Lachrymation. The substance is irritating to the eyes, skin and respiratory tract. See Notes.

STOT-repeated exposure

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

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation 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

no data available

Bioaccumulative potential

An estimated BCF of 50 was calculated in fish for cyclohexylisocyanate(SRC), using an estimated log Kow of 3.06(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(SRC). However, the rapid hydrolysis of cyclohexylisocyanated precludes bioconcentration(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of cyclohexylisocyanate can be estimated to be 800(SRC). According to a classification scheme(2), this estimated Koc value suggests that cyclohexylisocyanate is expected to have low mobility 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: UN2488 (For reference only, please check.)

IMDG: UN2488 (For reference only, please check.)

IATA: UN2488 (For reference only, please check.)

UN Proper Shipping Name

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

IMDG: CYCLOHEXYL ISOCYANATE (For reference only, please check.)

IATA: CYCLOHEXYL ISOCYANATE (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: 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>
Chemical Book

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?pagelD=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

Depending on the degree of exposure, periodic medical examination is suggested. The symptoms of asthma often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation are therefore essential. Anyone who has shown symptoms of asthma due to this substance should avoid all further contact with this substance. Insufficient data are available on the effect of this substance on human health, therefore utmost care must be taken.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.