ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

Cyclohexanecarbonyl isothiocyanate

Revision Date:2026-11-14 Revision Number:1

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

Product identifier

Product name	: Cyclohexanecarbonyl isothiocyanate
CBnumber	: CB61492004
CAS	: 27699-51-0
Synonyms	: Cyclohexanecarbonyl isothiocyanate (9CI)

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

GHS Label elements, including precautionary statements

Symbol(GHS)	No data available
Signal word	No data available

Precautionary statements

No data available

Hazard statements

No data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: Cyclohexanecarbonyl isothiocyanate
Synonyms	: Cyclohexanecarbonyl isothiocyanate (9CI)
CAS	: 27699-51-0
MF	: C8H11NOS
MW	: 169.24

SECTION 4: First aid measures

First Aid Measures

General advice

Consult a physician if necessary. Remove to fresh air.

Eye contact

Wash with plenty of water.

Skin Contact

Wash skin with soap and water.

Inhalation

Remove to fresh air If breathing is difficult, give oxygen If not breathing, give artificial respiration

Ingestion

Never give anything by mouth to an unconscious person. Clean mouth with water.

Most important symptoms and effects, both acute and delayed

Symptoms

No information available.

Indication of any immediate medical attention and special treatment needed

Note to physicians

Treat symptomatically.

SECTION 5: Firefighting measures

Suitable Extinguishing Media

Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable Extinguishing Media

None.

Specific hazards arising from the chemical

Specific hazards arising from the chemical

No information available.

Hazardous combustion products

Hydrogen cyanide. Hydrogen sulfide. Carbon oxides. Nitrogen oxides (NOx).

Explosion data

Sensitivity to Mechanical Impact

No information available.

Sensitivity to Static Discharge

No information available.

Protective equipment and precautions for firefighters

Protective equipment and precautions for firefighters

As in any fire, wear self contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal precautions

Ensure adequate ventilation, especially in confined areas.

Environmental precautions

Environmental precautions

See Section 12 for additional Ecological Information.

Methods and material for containment and cleaning up

Methods for containment

Prevent further leakage or spillage if safe to do so.

Methods for cleaning up

Use personal protective equipment as required. Cover powder spill with plastic sheet or tarp to minimize spreading and keep powder dry. Take up mechanically, placing in appropriate containers for disposal. Avoid creating dust. Clean contaminated surface thoroughly.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Handle in accordance with good industrial hygiene and safety practice.

Conditions for safe storage, including any incompatibilities

Storage Conditions

Keep containers tightly closed in a dry, cool and well-ventilated place. Store at 4 °C.

Incompatible materials

None known based on information supplied.

SECTION 8: Exposure controls/personal protection

Control parameters

Exposure Guidelines

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Appropriate engineering controls

Engineering Controls

Showers

Eyewash stations

Ventilation systems

Individual protection measures, such as personal protective equipment

Eye/face protection

Wear safety glasses with side shields (or goggles).

Skin and Body Protection

Wear protective gloves and protective clothing.

Respiratory protection

If exposure limits are exceeded or irritation is experienced, NIOSH/MSHA approved respiratory protection should be worn. Positive-pressure supplied air respirators may be required for high airborne contaminant concentrations. Respiratory protection must be provided in accordance with current local regulations.

General Hygiene Considerations

Handle in accordance with good industrial hygiene and safety practice.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical State	liquid
Appearance	No information available
Odor	No information available
pH	No information available
Melting point/freezing point	76.69 °C
Boiling point	248.4±7.0 °C(Predicted)
Flash point	No information available
Density	1.18±0.1 g/cm3(Predicted)
Evaporation rate	No information available
Upper flammability limits	No information available
Lower flammability limit	No information available
Vapor pressure	No information available
Vapor density	No information available
Specific gravity	No information available
Water solubility	No information available
Solubility in other solvents	No information available
Partition coefficient	No information available
Autoignition temperature	No information available
Decomposition temperature	No information available
Kinematic viscosity	No information available
Explosive properties	No information available
Oxidizing properties	No information available

SECTION 10: Stability and reactivity

Reactivity

Not applicable

Chemical stability

Stable under recommended storage conditions.

Possibility of Hazardous Reactions

Contact with acids may liberate toxic gas.

Hazardous polymerization

No information available.

Conditions to avoid

Extremes of temperature and direct sunlight.

Incompatible materials

Strong oxidizing agents.

Hazardous Decomposition Products

Hydrogen cyanide. Hydrogen sulfide. Carbon oxides. Nitrogen oxides (NOx).

SECTION 11: Toxicological information

Information on likely routes of exposure

Inhalation

No data available.

Eye contact

No data available.

Skin Contact

No data available.

Ingestion

No data available.

Information on toxicological effects

Symptoms

No information available.

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Chronic Toxicity

No information available.

Numerical measures of toxicity - Product Information

Unknown acute toxicity

100% of the mixture consists of ingredient(s) of unknown toxicity

SECTION 12: Ecological information

Ecotoxicity

May cause long lasting harmful effects to aquatic life

100% of the mixture consists of components(s) of unknown hazards to the aquatic environment.

Persistence and degradability

No information available.

Bioaccumulation

No information available.

Mobility

No information available.

SECTION 13: Disposal considerations

Disposal of wastes

Disposal should be in accordance with applicable regional, national and local laws and regulations.

Contaminated packaging

Do not reuse container.

SECTION 14: Transport information

DOT

Not regulated

IMDG

Not regulated

IATA

Not regulated

SECTION 15: Regulatory information

International Inventories

All of the components in the product are on the following Inventory lists

X - Listed

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

EINECS/ELINCS - European Inventory of Existing Chemical Substances/European List of Notified Chemical Substances

ENCS - Japan Existing and New Chemical Substances

IECSC - China Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

US Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372.

SARA 311/312 Hazard Categories

Acute health hazard

No

Chronic Health Hazard

No

Fire hazard

No

Sudden release of pressure hazard

No

Reactive hazard

No

CWA (Clean Water Act)

This product does not contain any substances regulated as pollutants pursuant to the Clean Water Act (40 CFR 122.21 and 40 CFR 122.42).

US State Regulations

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

This product does not contain any substances regulated by state right-to-know regulations

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.