



ISO PHORONE DI-ISO-CYANATE
CAS NO 4098-71-9

MATERIAL SAFETY DATA SHEET
SDS/MSDS

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

1.1 Product identifiers

Product name : Iso Phorone Di-Iso-Cyanate

CAS-No. : 4098-71-9

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

Identified uses : Laboratory chemicals, Industrial & for professional use only.

1.3 Details of the supplier of the safety data sheet

Company : Central Drug House (P) Ltd
7/28 Vardaan House
Ansari Road Daryaganj
New Delhi -110002
INDIA

Telephone : +91 11 49404040

Email : care@cdhfinechemical.com

1.4 Emergency telephone number

Emergency Phone # : +91 11 49404040 (9:00am - 6:00 pm) [Office hours]

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Acute toxicity, Inhalation (Category 1), H330

Skin irritation (Category 2), H315

Eye irritation (Category 2), H319

Respiratory sensitization (Category 1), H334

Skin sensitization (Category 1), H317

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Long-term (chronic) aquatic hazard (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal Word

Danger

Hazard statement(s)

H315

Causes skin irritation.

H317

May cause an allergic skin reaction.

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.

H411

Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P260

Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.

P273

Avoid release to the environment.

P280

Wear protective gloves/ eye protection/ face protection.

P302 + P352

IF ON SKIN: Wash with plenty of water.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard Statements

none

"As from 24 August 2023 adequate training is required before industrial or professional use."

Reduced Labeling (<= 125 ml)

Pictogram



Signal Word

Danger

Hazard statement(s)

H330

Fatal if inhaled.

H334

May cause allergy or asthma symptoms or breathing difficulties if inhaled.

H317

May cause an allergic skin reaction.

Precautionary statement(s)

P260

Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.

P302 + P352

IF ON SKIN: Wash with plenty of water.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

Supplemental Hazard Statements

none

2.2 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.
Lachrymator.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : 5-Isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane

Formula : C₁₂H₁₈N₂O₂

Molecular weight : 222,28 g/mol

CAS-No. : 4098-71-9

EC-No. : 223-861-6

Index-No. : 615-008-00-5

Component	Classification	Concentration
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate		
CAS-No. 4098-71-9 EC-No. 223-861-6 Index-No. 615-008-00-5	Acute Tox. 1; Skin Irrit. 2; Eye Irrit. 2; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; Aquatic Chronic 2; H330, H315, H319, H334, H317, H335, H411 Concentration limits: >= 0,5 %: Resp. Sens. 1, H334; >= 0,5 %: Skin Sens. 1, H317;	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Foam Water

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Moisture sensitive.

Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Respiratory protection

Recommended Filter type: Filter B-(P2)

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties

- | | |
|---|--|
| a) Physical state | liquid |
| b) Color | light yellow |
| c) Odor | pungent |
| d) Melting point/freezing point | Melting point/freezing point: -60 °C - (ECHA) |
| e) Initial boiling point and boiling range | 158 - 159 °C at 20 hPa - lit. |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | No data available |
| h) Flash point | 163 °C - closed cup |
| i) Autoignition temperature | 430 °C at 1.013 hPa |
| j) Decomposition temperature | No data available |
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: 14,2 mPa.s at 20 °C - OECD Test Guideline 114 |
| m) Water solubility | ca.0,015 g/l at 23 °C - OECD Test Guideline 105 |
| n) Partition coefficient: n-octanol/water | log Pow: 0,99 at 23 °C - OECD Test Guideline 107 - Bioaccumulation is not expected. |
| o) Vapor pressure | < 0,1 hPa at 20 °C - OECD Test Guideline 104 |
| p) Density | 1,049 g/cm ³ at 25 °C - lit. |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Alcohols
amides
Amines
Oxidizing agents
Ammonia
alkali hydroxides
glycol
phenol
urea
Water
mercaptans

10.4 Conditions to avoid

Avoid moisture.

Strong heating.

10.5 Incompatible materials

Metals

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 4.814 mg/kg

(OECD Test Guideline 401)

Acute toxicity estimate Inhalation - 4 h - 0,0051 mg/l - vapor(Expert judgment)

LC50 Inhalation - Rat - male and female - 4 h - 0,04 mg/l - aerosol

(OECD Test Guideline 403)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Acute toxicity estimate Inhalation - 4 h - 0,0051 mg/l - vapor

(Expert judgment)

LD50 Dermal - Rat - male and female - > 7.000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

(Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Causes sensitization.

May cause sensitization by skin contact.

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Chromosome aberration test in vitro

Species: Mouse

Application Route: inhalation (vapor)

Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information**Endocrine disrupting properties****Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

RTECS: NQ9370000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	static test LC50 - Cyprinus carpio (Carp) - > 208 mg/l - 96,0 h (Regulation (EC) No. 440/2008, Annex, C.1)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 27 mg/l - 48 h (Regulation (EC) No. 440/2008, Annex, C.2)
Toxicity to algae	static test NOEC - Desmodesmus subspicatus (green algae) - 4,4 mg/l - 72 h (Regulation (EC) No. 440/2008, Annex, C.3) static test EC50 - Desmodesmus subspicatus (green algae) - > 70 mg/l - 72 h (Regulation (EC) No. 440/2008, Annex, C.3)
Toxicity to bacteria	static test EC50 - activated sludge - 263 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 0 % - Not readily biodegradable. (Regulation (EC) No. 440/2008, Annex, C.4-D)
------------------	--

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2290

IMDG: 2290

IATA: 2290

14.2 UN proper shipping name

ADR/RID: ISOPHORONE DIISOCYANATE

IMDG: ISOPHORONE DIISOCYANATE

IATA: Isophorone diisocyanate

14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA: 6.1

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: no

14.6 Special precautions for user

No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Authorisations and/or restrictions on use

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII)

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

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

: ENVIRONMENTAL HAZARDS
: ACUTE TOXIC
: ENVIRONMENTAL HAZARDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
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.
H411	Toxic to aquatic life with long lasting effects.

Further information

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. Central Drug House (P) Ltd and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.cdhfinechemical.com for additional terms and conditions of sale.