

## SAFETY DATA SHEET

Issue Date 14-Apr-2025  
Revision Number 3.05

## 1. IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND OF THE COMPANY/UNDERTAKING

Product identifier

**Product Name** 3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate(mixture of isomers)

Other means of identification

**Product Code(s)** 090-03022,094-03025

Recommended use of the chemical and restrictions on use

**Recommended Use** For research use only.

**Uses advised against** Seek expert judgment when using for purposes other than those recommended.

Details of the supplier of the safety data sheet**Manufacturer Address**

FUJIFILM Wako Pure Chemical Corporation  
1-2, Doshomachi 3-Chome,

Chuo-ku Osaka 540-8605, Japan

Tel : +81-6-6203-3741

Fax: +81-6-6201-5964

**Distributor**

FUJIFILM Irvine Scientific  
E. Warner Avenue, Santa Ana, CA 92705-5505, U.S.A.: +1 949 261 7800  
Fax: +1 949 261 6522

## 2. HAZARDS IDENTIFICATION

**GHS classification**Classification of the substance or mixture

**Acute toxicity - Inhalation (Dusts/Mists)**

Category 1

**Skin corrosion/irritation**

Category 1 A

**Serious eye damage/eye irritation**

Category 2A

**Respiratory sensitization**

Category 1

**Skin sensitization**

Category 1

**Specific target organ toxicity (single exposure)**

Category 1

Category 1 respiratory system

**Specific target organ toxicity (repeated exposure)**

Category 1

Category 1 respiratory system

**Acute aquatic toxicity**

Category 3

**Chronic aquatic toxicity**

Category 3

**Pictograms**

Signal word



Danger

**Hazard statements**

H314 - Causes severe skin burns and eye damage

H319 - Causes serious eye irritation

H330 - Fatal if inhaled

H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled

H317 - May cause an allergic skin reaction

H402 - Harmful to aquatic life

H412 - Harmful to aquatic life with long lasting effects

H370 - Causes damage to the following organs: respiratory system

H372 - Causes damage to the following organs through prolonged or repeated exposure: respiratory system

**Precautionary statements-(Prevention)**

Do not breathe dust/fume/gas/mist/vapors/spray Wash face, hands and any exposed skin thoroughly after handling Wear protective gloves/protective clothing/eye protection/face protection In case of inadequate ventilation wear respiratory protection Contaminated work clothing should not be allowed out of the workplace Do not eat, drink or smoke when using this product Avoid release to the environment

**Precautionary statements-(Response)**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing Immediately call a POISON CENTER or doctor/physician  
 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower Wash contaminated clothing before reuse If skin irritation or rash occurs: Get medical advice/attention  
 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting

**Precautionary statements-(Storage)**

Store locked up

**Precautionary statements-(Disposal)**

Dispose of contents/container to an approved waste disposal plant

**Others**

**Other hazards** Not available

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

**Single Substance or Mixture** Substance

**Formula** C12H18N2O2

Chemical Name	Molecular weight	CAS RN	Weight-%
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	222.28	4098-71-9	98.0

**Impurities and/or Additives:** Not applicable

**Substances Remarks:** This product is composed of isomer mixture.

### 4. FIRST AID MEASURES

**First aid measures**

**Eye contact** Rinse thoroughly with plenty of water for at least 15 minutes, lifting lower and upper eyelids. Consult a physician.

**Skin contact** Wash skin with soap and water.

**Inhalation** Remove to fresh air.

**Ingestion** Rinse mouth. Never give anything by mouth to an unconscious person. Call a physician or poison control center immediately. Do not induce vomiting without medical advice.

**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.

### 5. FIRE-FIGHTING MEASURES

**Suitable Extinguishing media**

Carbon dioxide (CO<sub>2</sub>). Foam. Extinguishing powder. Sand.

**Specific hazards arising from the chemical**

Thermal decomposition can lead to release of irritating and toxic gases and vapors.

**Explosion data**

**Sensitivity to Mechanical Impact** none.  
**Sensitivity to Static Discharge** none.

**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.

## 6. ACCIDENTAL RELEASE MEASURES

**Personal precautions, protective equipment and emergency procedures**

**Personal precautions, protective equipment and emergency procedures** 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 and material for containment and cleaning up** Absorb dry sand, earth, sawdust and the waste. Collect empty container that can be sealed.

**Methods for cleaning up** Pick up and transfer to properly labeled containers.

## 7. HANDLING AND STORAGE

**Precautions for safe handling**

**Technical measures** Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Use with local exhaust ventilation.

**Protective measures** Handle in accordance with good industrial hygiene and safety practice.

**Conditions for safe storage, including any incompatibilities**

**Storage conditions** Keep container protect from light, store in well-ventilated place at room temperature (preferably cool). Keep container tightly closed. Store locked up.

**Packaging materials** Glass.

**Incompatible materials** Strong oxidizing agents.

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

**Engineering controls**

In case of indoor workplace, seal the source or use a local exhaust system. Provide the safety shower facility, and hand- and eye-wash facility. And display their position clearly.

**Exposure limits**

Chemical Name	ACGIH	OSHA PEL	NIOSH IDLH
3-Isocyanatomethyl-3,5,5-trime	TWA: 0.005 ppm	(vacated) TWA: 0.005 ppm	TWA: 0.005 ppm

thylcyclohexyl Isocyanate 4098-71-9		(vacated) STEL: 0.02 ppm (vacated) S*	TWA: 0.045 mg/m <sup>3</sup> STEL: 0.02 ppm STEL: 0.180 mg/m <sup>3</sup>
--	--	--	---

**Personal protective equipment**

<b>Respiratory protection</b>	Protective mask
<b>Hand protection</b>	chemical protective gloves ( JIS T 8116 )
<b>Eye protection</b>	protective eyeglasses or chemical safety goggles (JIS T 8147)
<b>Skin and body protection</b>	Long-sleeved work clothes

**General hygiene considerations**

Handle in accordance with good industrial hygiene and safety practice.

**9. PHYSICAL AND CHEMICAL PROPERTIES****Form****Color****Turbidity****Appearance****Odor****pH****Melting point/freezing point****Boiling point, initial boiling point and boiling range****Flash point****Evaporation rate:****Flammability (solid, gas):****Upper/lower flammability or explosive limits****Upper:****Lower:****Vapour pressure****Vapour density****Specific Gravity / Relative density****Solubilities****n-Octanol/water partition coefficient:(log Pow)****Auto-ignition temperature:****Decomposition temperature:****Viscosity (coefficient of viscosity)****Dynamic viscosity****Particle characteristics**

Colorless - slightly yellow

clear

liquid

no data available

no data available

- 60 °C

no data available

162 °C

no data available

no data available

no data available

no data available

0.0004 hPa

7.7 (air = 1)

1.059 - 1.067 g/mL

Ethanol and acetone : freely soluble . water : practically insoluble,or insoluble .

no data available

**10. STABILITY AND REACTIVITY****Stability****Chemical stability****Reactivity**

May be altered by light.

no data available

**Hazardous reactions**

Reacts violently with acids, may cause fire or explosion. Reacts with bases to produce toxic gas.

**Conditions to avoid**

Extremes of temperature and direct sunlight, Heat, flames and sparks, static electricity, spark

**Incompatible materials**

Strong oxidizing agents

**Hazardous decomposition products**Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>)**11. TOXICOLOGICAL INFORMATION**

**Acute toxicity**

Chemical Name	Oral LD50	Dermal LD50	Inhalation LC50
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	>2,645 mg/kg ( Rat )	>7,000 mg/kg ( Rat )	0.04 mg/L ( Rat ) 4 h

Chemical Name	Acute toxicity -oral- source information	Acute toxicity -dermal- source information	Acute toxicity -inhalation gas-source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.

Chemical Name	Acute toxicity -inhalation vapor- source information	Acute toxicity -inhalation dust- source information	Acute toxicity -inhalation mist- source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.

**Skin irritation/corrosion**

Chemical Name	Skin corrosion/irritation source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**Serious eye damage/ irritation**

Chemical Name	Serious eye damage/irritation source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**Respiratory or skin sensitization**

Chemical Name	Respiratory or Skin sensitization source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**Reproductive cell mutagenicity**

Chemical Name	germ cell mutagenicity source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**Carcinogenicity**

Chemical Name	Carcinogenicity source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**Reproductive toxicity**

Chemical Name	Reproductive toxicity source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**STOT-single exposure**

Chemical Name	STOT -single exposure- source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**STOT-repeated exposure**

Chemical Name	STOT -repeated exposure- source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**Aspiration hazard**

Chemical Name	Aspiration Hazard source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.

**12. ECOLOGICAL INFORMATION****Ecotoxicity**

Chemical Name	Algae/aquatic plants	Fish	Toxicity to microorganisms	Crustacea
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate 4098-71-9	EC50 : Desmodesmus subspicatus 118.7 mg/L 72 h	N/A	N/A	EC50 : Daphnia magna 83.7 mg/L 24 h

**Persistence and degradability**

No information available

**Bioaccumulative potential**

No information available

**Mobility**

no data available

**Mobility in soil**

No information available

**Other Data**

No information available

**13. DISPOSAL CONSIDERATIONS****Waste treatment methods**

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

**Precautionary including method of disposing contaminated packaging** Disposal should be in accordance with applicable regional, national and local laws and regulations.

**14. TRANSPORT INFORMATION****DOT**

**UN/ID No** UN2290  
**Proper shipping name:** Isophorone diisocyanate  
**UN classification** 6.1  
**Subsidiary hazard class**  
**Packing group** III  
**Marine pollutant** Not applicable

**IATA**

**UN/ID No** UN2290  
**Proper shipping name:** Isophorone diisocyanate  
**UN classification** 6.1  
**Subsidiary hazard class**  
**Packing group** III  
**Environmentally Hazardous Substance** Not applicable

**IMDG**

**UN/ID No** UN2290  
**Proper shipping name:** Isophorone diisocyanate  
**UN classification** 6.1  
**Subsidiary hazard class**  
**Packing group** III  
**Marine pollutant (Sea)** Not applicable

**15. REGULATORY INFORMATION****US Federal Regulations****SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product contains a chemical or chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

Chemical Name	CAS RN	Weight-%	SARA 313 - Threshold Values %
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate - 4098-71-9	4098-71-9	98.0	1.0

**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)

**CERCLA**

This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302)

Chemical Name	Hazardous Substances RQs	CERCLA/SARA RQ	Reportable Quantity (RQ)
3-Isocyanatomethyl-3,5,5-trimethyl cyclohexyl Isocyanate 4098-71-9	N/A	500 lb	N/A

**US State Regulations****California Proposition 65**

This product does not contain any chemicals regulated by Proposition 65

**U.S. State Right-to-Know Regulations**

Chemical Name	New Jersey	Massachusetts	Pennsylvania
3-Isocyanatomethyl-3,5,5-trimethyl cyclohexyl Isocyanate 4098-71-9	X	X	X

**U.S. EPA Label Information**

EPA Pesticide Registration Number Not applicable

**16. OTHER INFORMATION**

**Issue Date** 09-Apr-2025

**Issue Date** 14-Apr-2025

**Revision Note**

No information available

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text.

**End of Safety Data Sheet**