

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
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 Chuo-ku Osaka 540-8605, Japan
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Distributor

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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 (CO₂). 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 none.

Impact

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 ³ STEL: 0.02 ppm STEL: 0.180 mg/m ³
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Personal protective equipment**Respiratory protection**

Protective mask

Hand protection

chemical protective gloves (JIS T 8116)

Eye protection

protective eyeglasses or chemical safety goggles (JIS T 8147)

Skin and body protection

Long-sleeved work clothes

General hygiene considerations

Handle in accordance with good industrial hygiene and safety practice.

9. PHYSICAL AND CHEMICAL PROPERTIES

Form**Color**

Colorless - slightly yellow

Turbidity

clear

Appearance

liquid

Odor

no data available

pH

no data available

Melting point/freezing point

- 60 °C

Boiling point, initial boiling point and boiling range

no data available

Flash point

162 °C

Evaporation rate:

no data available

Flammability (solid, gas):

no data available

Upper/lower flammability or explosive limits**Upper:**

no data available

Lower:

no data available

Vapour pressure

0.0004 hPa

Vapour density

7.7 (air = 1)

Specific Gravity / Relative density

1.059 - 1.067 g/mL

Solubilities

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

n-Octanol/water partition coefficient:(log Pow)

no data available

Auto-ignition temperature:

no data available

Decomposition temperature:

no data available

Viscosity (coefficient of viscosity)

no data available

Dynamic viscosity

no data available

Particle characteristics

no data available

10. STABILITY AND REACTIVITY

Stability**Chemical stability**

May be altered by light.

Reactivity

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 productsCarbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x)

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

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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