

SAFETY DATA SHEET

According to JIS Z 7253:2019
Revision date 26-Feb-2024
 Revision Number 4.05

Section 1: PRODUCT AND COMPANY IDENTIFICATION

Product Name	3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate(mixture of isomers)
Product Code	090-03022,094-03025

Supplier	FUJIFILM Wako Pure Chemical Corporation 1-2 Doshomachi 3-Chome, Chuo-ku, Osaka 540-8605, Japan Phone: +81-6-6203-3741 Fax: +81-6-6203-2029
Emergency telephone number	+81-6-6203-3741 / +81-3-3270-8571
Recommended uses	For research use only
Restrictions on use	Seek expert judgment when using for purposes other than those recommended.

Section 2: HAZARDS IDENTIFICATION

GHS classification

Classification of the substance or mixture

Acute toxicity - Inhalation (Dusts/Mists)	Category 1
Skin corrosion/irritation	Category 1
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

Section 3: COMPOSITION/INFORMATION ON INGREDIENTS

Single Substance or Mixture Substance

Formula C₁₂H₁₈N₂O₂

Chemical Name	Weight-%	Molecular weight	ENCS	ISHL No.	CAS RN
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	98.0	222.28	(3)-2492	*	4098-71-9

Note on ISHL No.: * in the table means announced chemical substances.

Substances Remarks: This product is composed of isomer mixture.

Section 4: FIRST AID MEASURES

Inhalation

Remove to fresh air. If symptoms persist, call a physician.

Skin contact

Wash off immediately with soap and plenty of water. If symptoms persist, call a physician.

Eye contact

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

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.

Protection of first-aiders

Use personal protective equipment as required.

Section 5: FIRE FIGHTING MEASURES

Suitable extinguishing media

Water spray (fog), Carbon dioxide (CO₂), Foam, Extinguishing powder, Sand

Unsuitable extinguishing media

No information available

Specific hazards arising from the chemical product

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

Special extinguishing method

No information available

Special protective actions for fire-fighters

Use personal protective equipment as required. Firefighters should wear self-contained breathing apparatus and full firefighting turnout gear.

Section 6: ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures

For indoor, provide adequate ventilation process until the end of working. Deny unnecessary entry other than the people involved by, for example, using a rope. While working, wear appropriate protective equipments to avoid adhering it on skin, or inhaling the gas. Work from windward, and retract the people downwind.

Environmental precautions

To be careful not discharged to the environment without being properly handled waste water contaminated.

Methods and materials for contaminant and methods and materials for cleaning up

Absorb dry sand, earth, sawdust and the waste. Collect empty container that can be sealed.

Recovery, neutralization

No information available

Secondary disaster prevention measures

Clean contaminated objects and areas thoroughly observing environmental regulations.

Section 7: HANDLING AND STORAGE

Handling**Technical measures**

Highly flammable. Avoid contact with high temperature objects, spark, and strong oxidizing agents. Use with local exhaust ventilation.

Precautions

Do not rough handling containers, such as upsetting, falling, giving a shock, and dragging. Prevent leakage, overflow, and scattering. Not to generate steam and dust in vain. Seal the container after use. After handling, wash hands and face, and then gargle. In places other than those specified, should not be smoking or eating and drinking. Should not be brought contaminated protective equipment and gloves to rest stops. Deny unnecessary entry of non-emergency personnel to the handling area.

Safety handling precautions

Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapors). Use personal protective equipment as required. Avoid contact with skin, eyes or clothing.

Storage**Safe storage conditions****Storage conditions**

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

Safe packaging material

Glass

Incompatible substances

Strong oxidizing agents

Section 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	JSOH (Japan)	ISHL (Japan)	ACGIH
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate 4098-71-9	N/A	N/A	TWA: 0.005 ppm

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.

If this product is classified as "Chemical Substances Hazardous to Skin, etc.", use appropriate protective equipment to them.

Section 9: PHYSICAL AND CHEMICAL PROPERTIES**Form****Color**

Colorless - slightly yellow

Turbidity

clear

Appearance

liquid

Odor

no data available

Melting point/freezing point

-60 °C

Boiling point, initial boiling point and boiling range

no data available

Flammability

no data available

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

Flash point

162 °C

Auto-ignition temperature:

no data available

Decomposition temperature:

no data available

pH

no data available

Viscosity (coefficient of viscosity)

no data available

Dynamic viscosity

no data available

Solubilities

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

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

no data available

Vapour pressure

0.0004 hPa

Specific Gravity / Relative density

1.059 - 1.067 g/mL

Vapour density

7.7 (air = 1)

Particle characteristics

no data available

Section 10: STABILITY AND REACTIVITY**Stability****Reactivity**

no data available

Chemical stability

May be altered by light.

Hazardous reactions

None under normal processing

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)**Section 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)	0.135 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.

Section 12: ECOLOGICAL INFORMATION**Ecotoxicity**

Chemical Name	Algae/aquatic plants	Fish	Crustacea
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	EC50 : <i>Desmodesmus</i>	LC50: <i>Leuciscus idus</i>	EC50 : <i>Daphnia magna</i>

thylcyclohexyl Isocyanate	<i>subspicatus</i> 118.7 mg/L 72 h	1.8 mg/L 48 h	83.7 mg/L 24 h
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Other data

Chemical Name	Short-term (acute) hazardous to the aquatic environment source information	Long-term (chronic) hazardous to the aquatic environment source information
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate	Based on the NITE GHS classification results.	Based on the NITE GHS classification results.

Persistence and degradability	No information available
Bioaccumulative potential	No information available
Mobility in soil	No information available
Hazard to the ozone layer	No information available

Section 13: DISPOSAL CONSIDERATIONS

Waste from residues

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

Contaminated container and contaminated packaging

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

Section 14: TRANSPORT INFORMATION

ADR/RID

UN number	UN2290
Proper shipping name:	Isophorone diisocyanate
UN classification	6.1
Subsidiary hazard class	
Packing group	III
Marine pollutant	Not applicable

IMDG

UN number	UN2290
Proper shipping name:	Isophorone diisocyanate
UN classification	6.1
Subsidiary hazard class	
Packing group	III
Marine pollutant (Sea)	Not applicable
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	No information available

IATA

UN number	UN2290
Proper shipping name:	Isophorone diisocyanate
UN classification	6.1
Subsidiary hazard class	
Packing group	III
Environmentally Hazardous Substance	Not applicable

Section 15: REGULATORY INFORMATION

Japanese regulations

Fire Service Act	Category IV, Class III petroleums, dangerous grade 3
Poisonous and Deleterious Substances Control Law	Poisonous Substances 2nd. Grade
Industrial Safety and Health Act	Notifiable Substances (Law Art.57-2)

Industrial Safety and Health Act (2024-)	Harmful Substances Whose Names Are to be Indicated on the Label (Law Art.57) 【2024.4.1~】 Chemical Substances Hazardous to Skin, etc.(Regulations Article 594-2 Paragraph 1)
Regulations for the carriage and storage of dangerous goods in ship	Toxic Substances - Poison (Ordinance Art.3, Ministry of Transportation Ordinance Regarding Transport by Ship and Storage, Attached Table 1)
Civil Aeronautics Law	Toxic and Infectious Substances (Ordinance Art.194, MITL Notification for Air Transportation of Explosives etc., Attached Table 1)
Pollutant Release and Transfer Register Law (2023.4.1-)	Class 1
Class 1 - No.	34
Export Trade Control Order	Not applicable
Air Pollution Control Law	Hazardous Air Pollutants

Chemical Name	Poisonous and Deleterious Substances Control Law	Industrial Safety and Health Act Substances (Law Art.57-2)	Pollutant Release and Transfer Register Law (2023.4.1-)
3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl Isocyanate 4098-71-9 (98.0)	Applicable	Applicable	Applicable

Section 16: OTHER INFORMATION

Key literature references and sources for data etc.

NITE: National Institute of Technology and Evaluation (JAPAN)
<http://www.safe.nite.go.jp/japan/db.html>
 IATA dangerous Goods Regulations
 RTECS:Registry of Toxic Effects of Chemical Substances
 Japan Industrial Safety and Health Association GHS Model SDS
 Dictionary of Synthetic Organic Chemistry , SSOCJ, Koudansha Scientific Co.Ltd.
 Chemical Dictionary, Kyouritsu Publishing Co., Ltd.
 etc

Record of SDS revisions Disclaimer

The following contents were revised. Regulatory information.

This SDS is according to JIS Z 7253: 2019. 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, 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.

GHS Classification is according to JIS Z 7252:2019. *JIS: Japanese Industrial Standards

End of Safety Data Sheet