

Safety Data Sheet

Isophorone diisocyanate

Version : V2.0.0.1

Report No. : BWJ5448-2016-MSDS-US

Creation Date : 2025/10/16

Revision Date : -



*Prepared according to American OSHA HCS-2024 (29 CFR 1910.1200)

1 Identification

Product identifier

Product Name	Isophorone diisocyanate
Cat No.	BWJ5448-2016
CAS No.	4098-71-9
EC No.	223-861-6
Molecular Formula	C ₁₂ H ₁₈ N ₂ O ₂

Recommended use of the product and restrictions on use

Relevant identified uses	Please consult manufacturer.
Uses advised against	Please consult manufacturer.

Details of the supplier of the Safety Data Sheet

Name of the company	Weiyel Inc
Address of the company	Hedian Light Industrial Park, Chengguan Town, Shangcheng County, Xinyang City, Henan Province, China
Post code	465350
Telephone number	010-58103678
Fax number	010-84840368
E-mail address	info@weiyel.com

Emergency phone number

Emergency phone number	010-58103678
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2 Hazard(s) identification

Hazard classification according to 29 CFR 1910.1200

Skin Corrosion/Irritation	Category 2
Sensitization - skin	Category 1
Serious eye damage/irritation	Category 2
Acute Toxicity - Inhalation	Category 1
Sensitization - respiratory	Category 1
Specific target organ toxicity - single exposure; respiratory tract irritation	Category 3

Label elements

Hazard pictograms	  
Signal word	Danger

Hazard statements

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

Precautionary statements

◆ Prevention

P260	Do not breathe dust/fume.
P264	Wash hands and other parts of the body (if related) thoroughly after handling.
P271	Use only outdoors or with adequate ventilation.
P272	Contaminated work clothing should not be allowed out of the workplace.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P284	In case of inadequate ventilation wear respiratory protection.

◆ Response

P320	Specific treatment is urgent (see related instructions on the label).
P321	Specific treatment (see related instructions on the label).
P302+P352	IF ON SKIN: Wash with plenty of water.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P362+P364	Take off contaminated clothing and wash it before reuse.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

◆ Storage

P405	Store locked up.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.

◆ Disposal

P501	Dispose of contents/container in accordance with local/regional/national/international regulations.
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Other hazards

	Not applicable.
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Hazard description

◆ Physical and chemical hazards

	No information available
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◆ Health hazards

Inhaled	Cough. Sore throat. Burning sensation.
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Ingestion	Sore throat. Burning sensation. Abdominal pain.
Skin Contact	Redness. Pain. Serious skin burns.
Eye	Redness. Pain.

◆ Environmental hazards

	Please refer to 12th chapter of SDS.
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3 Composition/information on ingredients

| Substance/mixture

	Substance
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Component	CAS No.	EC No.	Concentration (wt, %)
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4098-71-9	223-861-6	99.89

4 First-aid measures

| Description of first aid measures

General advice	Immediate medical attention is required. Show this safety data sheet (SDS) to the doctor in attendance.
Eye contact	Rinse with plenty of water (remove contact lenses if easily possible). Refer immediately for medical attention.
Skin contact	Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention.
Ingestion	Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink. Refer for medical attention.
Inhalation	Fresh air, rest. Half-upright position. Refer immediately for medical attention.
Protecting of first-aiders	Ensure that medical personnel are aware of the substance involved. Take precautions to protect themselves and prevent spread of contamination.

| Most important symptoms/effects, acute and delayed

1	Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.
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| Indication of any immediate medical attention and special treatment needed

1	Treat symptomatically.
2	Symptoms may be delayed.

5 Fire-fighting measures

| Extinguishing media

Suitable extinguishing media	Small fire: CO ₂ , dry chemical, dry sand, alcohol-resistant foam; Large fire: water spray, fog or alcohol-resistant foam; Fire involving tanks, rail tank cars or highway tanks: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Do not get water inside containers.
Unsuitable extinguishing media	Large fire: avoid aiming straight or solid streams directly onto the product.

| Specific hazards arising from the substance or mixture

1	May emit poisonous fumes on fire.
2	Development of hazardous combustion gases or vapor possible in the event of fire.
3	May expansion or decompose explosively when heated or involved in fire.

| Special protective equipment and precautions for fire-fighters

1	As in any fire, wear self-contained breathing apparatus (MSHA/NIOSH approved or equivalent) and full protective gear.
2	Fight fire from a safe distance, with adequate cover.
3	Prevent fire extinguishing water from contaminating surface water or the ground water system.

6 Accidental release measures

| Personal precautions, protective equipment and emergency procedures

1	Fully encapsulating, vapor protective clothing should be worn for spills and leaks with no fire.
2	Do not touch or walk through spilled material.
3	Do not touch damaged containers or spilled material unless wearing appropriate protective clothing.
4	Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.
5	Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.
6	Use personal protective equipment, do not breathe dust/fume.

| Environmental precautions

1	Prevent further leakage or spillage if safe to do so.
2	Discharge into the environment must be avoided.

| Methods and materials for containment and cleaning up

1	Isolation of contaminated areas and restrictions on access.
2	It is recommended that emergency personnel wear dust masks and wear anti-virus suits.
3	Do not touch broken containers and spills before putting on appropriate protective clothing.
4	Cover the spill with a plastic sheet to reduce scattering.
5	Cut off the source of the leak as much as possible.
6	Keep leaks in a ventilated place.
7	It is recommended that emergency personnel wear dust masks.
8	Collect the spill with a clean shovel and place it in a clean, dry, loosely closed container and move the container away from the leak.
9	Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

7 Handling and storage

| Precautions for safe handling

1	Handling is performed in a well ventilated place.
2	Wear suitable protective equipment.
3	Avoid contact with skin and eyes.
4	Keep away from heat/sparks/open flames/ hot surfaces.

| Conditions for safe storage, including any incompatibilities

1	Keep containers tightly closed.
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2	Keep containers in a dry, cool and well-ventilated place.
3	Keep away from heat/sparks/open flames/hot surfaces.

8 Exposure controls/personal protection

Control parameters

◆ Occupational exposure limit values

Component	Country/Region	Limit value - Eight hours		Limit value - Short term	
		ppm	mg/m ³	ppm	mg/m ³
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	Permissible exposure standards for workers in the workplace	0.005	0.045	0.015	0.135
	Canada - Ontario	0.005	-	0.02	-
	USA - ACGIH	0.005	-	-	-
	USA - NIOSH	0.005	0.045	0.02	0.18
	Austria	0.01	0.09	0.02	0.18
	Belgium	0.005	0.046	-	-

Engineering controls

1	Ensure adequate ventilation, especially in confined areas.
2	Ensure that eyewash stations and safety showers are close to the workstation location.
3	Use explosion-proof electrical/ventilating/lighting/equipment.
4	Set up emergency exit and necessary risk-elimination area.

Personal protection equipment

General requirement	    
Eye protection	Must wear appropriate safety goggles.
Hand protection	Must wear appropriate chemical protective gloves.
Respiratory protection	Must wear appropriate personal dust proof gas mask.
Skin and body protection	Must wear appropriate chemical protective clothing and chemical resistant shoes.

9 Physical and chemical properties and safety characteristics

Physical and chemical properties

Appearance (physical state, color, etc.)	white or light yellow solid powder
Odor	No information available
Odor threshold	No information available
pH	No information available
Melting point/freezing point(°C)	-60
Initial boiling point and boiling range(°C)	158 (1.33kPa)

Flash point(Closed cup,°C)	155
Evaporation rate	Not applicable
Flammability	No information available
Upper/lower explosive limits[%(v/v)]	Upper limit : 4.5 ; Lower limit : 0.7
Vapor pressure	0.04Pa (20°C)
Vapor density(Air = 1)	> 1
Relative density(Water=1)	1.06
Solubility	15mg/L (23 °C)
n-octanol/water partition coefficient	4.75 (calculated)
Auto-ignition temperature(°C)	430
Decomposition temperature(°C)	310
Kinematic viscosity	Not applicable

10 Stability and reactivity

| Stability and reactivity

Reactivity	Contact with incompatible substances can cause decomposition or other chemical reactions.
Chemical stability	Stable under proper operation and storage conditions.
Possibility of hazardous reactions	No information available.
Conditions to avoid	Incompatible materials, heat, flame and spark.
Incompatible materials	No information available.
Hazardous decomposition products	Under normal conditions of storage and use, hazardous decomposition products should not be produced.

11 Toxicological information

| Acute toxicity

Component	LD ₅₀ (oral)	LD ₅₀ (dermal)	LC ₅₀ (inhalation,4h)
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4825mg/kg(Rat)	No information available	0.031mg/L(Rat)

| Carcinogenicity

Component	List of carcinogens by the IARC Monographs	Report on Carcinogens by NTP	OSHA Carcinogen List
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	Not Listed	Not Listed	Not Listed

| Others

3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate(Component)	
Skin corrosion/irritation	Causes skin irritation(Category 2)
Serious eye damage/irritation	Causes serious eye irritation(Category 2)
Skin sensitization	May cause an allergic skin reaction(Category 1)

Respiratory sensitization	May cause allergy or asthma symptoms or breathing difficulties if inhaled(Category 1)
Reproductive toxicity	Based on available data, the classification criteria are not met
STOT-single exposure	May cause respiratory irritation(Category 3)
STOT-repeated exposure	Based on available data, the classification criteria are not met
Aspiration hazard	Based on available data, the classification criteria are not met
Germ cell mutagenicity	Based on available data, the classification criteria are not met

12 Ecological information

| Acute aquatic toxicity

Acute aquatic toxicity	No information available
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| Chronic aquatic toxicity

Chronic aquatic toxicity	No information available
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| Persistence and degradability

Persistence and degradability	No information available
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| Bioaccumulative potential

Bioaccumulative potential	No information available
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| Mobility in soil

Component	log Koc	Remark
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4.562	

13 Disposal considerations

| Disposal considerations

Waste chemicals	Before disposal should refer to the relevant national and local laws and regulation. Recommend the use of incineration disposal.
Contaminated packaging	Containers may still present chemical hazard when empty. Keep away from hot and ignition source of fire. Return to supplier for recycling if possible.
Disposal recommendations	Refer to section waste chemicals and contaminated packaging.

14 Transport information

| Label and Mark

Transporting Label	
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| IMDG-CODE

UN number	2290
UN proper shipping name	ISOPHORONE DIISOCYANATE
Transport hazard class	6.1

Transport subsidiary hazard class	None
Packing group	III
Marine pollutant (Yes or no)	No

IATA-DGR

UN number	2290
UN proper shipping name	ISOPHORONE DII SOCYANATE
Transport hazard class	6.1
Transport subsidiary hazard class	None
Packing group	III

UN-ADR

UN number	2290
UN proper shipping name	ISOPHORONE DIISOCYANATE
Transport hazard class	6.1
Transport subsidiary hazard class	None
Packing group	III

Transport in bulk according to IMO instruments

- ◆ Transport in bulk according to Annex II of MARPOL and the IBC code

	Not Available
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- ◆ Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

	Not Available
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- ◆ Transport in bulk in accordance with the IGC Code

	Not Available
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Others

Precautions for transport	Transit should be anti-exposure, rain, high temperature. Strictly prohibited shipping or transportation with acids, alkalis, oxidants, food and food additives etc. Transport vehicles should be equipped with the appropriate variety and quantity of fire equipment and emergency equipment leakage during transport. Before transport, should be preceded by checking whether container integrity, sealing. The transport unit must be placarded and marked in accordance with relevant transporting requirements.
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15 Regulatory information

International chemical inventory

Component	A	B	C	D	E	F	G	H	I	J	K	L	M
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	√	√	√	√	√	√	√	√	√	√	√	√	√

- [A] China Inventory of Existing Chemical Substances(IECSC)
[B] European Inventory of Existing Commercial Chemical Substances(EC inventory)
[C] United States Toxic Substances Control Act Inventory(TSCA)
[D] Canadian Domestic Substances List(DSL)

- [E] New Zealand Inventory of Chemicals(NZIoC)
- [F] Philippines Inventory of Chemicals and Chemical Substances(PICCS)
- [G] Korea Existing Chemicals Inventory(KECL)
- [H] Australian. Inventory of Industrial Chemical (AIICS)
- [I] Japan Inventory of Existing & New Chemical Substances(ENCS)
- [J] Thailand Existing Chemicals Inventory(TECI)
- [K] Mexico National Inventory of Chemical Substances (INSQ)
- [L] Russia Inventory of Existing Substances(DRAFT)
- [M] Inventory of Existing Chemical Substances in Taiwan, China (TCSI)

List of Chemical Substances under International Conventions

Component	A	B	C
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	×	×	×

- [A] The Montreal Protocol on Substances that Deplete the Ozone Layer
- [B] Stockholm Convention on Persistent Organic Pollutants (POPs)
- [C] Rotterdam Convention on the prior informed consent procedure for certain hazardous chemicals and pesticides in international trade

US chemical inventory

Component	A	B	C	D	E	F	G	H
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	×	✓	×	✓	✓	✓	✓	×

- [A] US Clean Air Act (CAA)- Section 112, Hazardous Air Pollutants
- [B] US SARA 302- Extremely Hazardous Substance List
- [C] US CERCLA- Hazardous Substances List
- [D] US Massachusetts Right-to-Know Substance List
- [E] US New Jersey Right to Know Hazardous Substance List
- [F] US Pennsylvania Right to Know Hazardous Substance List
- [G] US New York City Right-to-Know Hazardous Substance List
- [H] US California Proposition 65 List

Note:

- “✓” Indicates that the substance included in the regulations.
- “×” No data or not included in the regulations.

16 Other information

Information on revision

Creation Date	2025/10/16
Revision Date	-
Reason for revision	-

Reference

- [1] IPCS: The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>.
- [2] IARC, website: <http://www.iarc.fr/>.
- [3] OECD: The Global Portal to Information on Chemical Substances, website: <https://www.echemportal.org/echemportal/>.
- [4] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>.
- [5] NLM: ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>.
- [6] EPA: Integrated Risk Information System, website: <http://cfpub.epa.gov/iris/>.
- [7] U.S. Department of Transportation: ERG, website: <http://www.phmsa.dot.gov/hazmat/library/erg>.
- [8] Germany GESTIS-database on hazard substance, website: <http://gestis-en.itrust.de/>.

Abbreviations and acronyms

CAS	Chemical Abstracts Service	UN	The United Nations
PC-STEL	Short term exposure limit	OECD	Organization for Economic Co-operation and Development
PC-TWA	Time Weighted Average	IMDG-CODE	International Maritime Dangerous Goods CODE
MAC	Maximum Allowable Concentration	IARC	International Agency for Research on Cancer
DNEL	Derived No Effect Level	ICAO	International Civil Aviation Organization
PNEC	Predicted No Effect Concentration	IATA	International Air Transportation Association
NOEC	No Observed Effect Concentration	ACGIH	American Conference of Governmental Industrial Hygienists
LC ₅₀	Lethal Concentration 50%	NFPA	National Fire Protection Association
LD ₅₀	Lethal Dose 50%	NTP	National Toxicology Program
EC ₅₀	Effective Concentration 50%	PBT	Persistent, Bioaccumulative, Toxic
EC _x	Effective Concentration X%	vPvB	very Persistent, very Bioaccumulative
P _{OW}	Partition coefficient Octanol: Water	CMR	Carcinogens, mutagens or substances toxic to reproduction
BCF	Bioconcentration factor	RPE	Respiratory Protective Equipment
ED	Endocrine disruptor	HCS	Hazard Communication Standard

Disclaimer

This Safety Data Sheet (SDS) was prepared according to OSHA HCS -2024. The data included was derived from international authoritative database and provided by the enterprise. Other information was based on the present state of our knowledge. We try to ensure the correctness of all information. However, due to the diversity of information sources and the limitations of our knowledge, this document is only for user's reference. Users should make their independent judgment of suitability of this information for their particular purposes. We do not assume responsibility for loss, damage or expense arising out of or in any way connected with the handling, storage, use or disposal of the product.