

SAFETY DATA SHEET

Creation Date 03-Sep-2009

Revision Date 29-Jul-2024

Revision Number 1

1. Identification

Product Name Isophorone diisocyanate

Cat No. : C42760

CAS No 4098-71-9
Synonyms 5-Isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute Inhalation Toxicity - Vapors	Category 1
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Respiratory Sensitization	Category 1
Skin Sensitization	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Danger

Hazard Statements

Causes skin irritation

Causes serious eye irritation

May cause an allergic skin reaction

Fatal if inhaled

May cause allergy or asthma symptoms or breathing difficulties if inhaled

May cause respiratory irritation

**Precautionary Statements****Prevention**

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

Use only outdoors or in a well-ventilated area

Wear respiratory protection

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

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Immediately call a POISON CENTER or doctor/physician

Call a POISON CENTER or doctor/physician if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water

Take off contaminated clothing and wash before reuse

If skin irritation or rash occurs: Get medical advice/attention

Eyes

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

If eye irritation persists: Get medical advice/attention

Storage

Store in a well-ventilated place. Keep container tightly closed

Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Toxic to aquatic life with long lasting effects

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Isophoronediiisocyanate	4098-71-9	<=100

4. First-aid measures

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Most important symptoms and effects	May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. None reasonably foreseeable. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	163 °C / 325.4 °F
Method -	No information available
Autoignition Temperature	430 °C / 806 °F
Explosion Limits	
Upper	4.5 vol %
Lower	0.7 vol %
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x).

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

NFPA

Health
4

Flammability
1

Instability
1

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.
Environmental Precautions	Do not flush into surface water or sanitary sewer system.
Methods for Containment and Clean Up	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

7. Handling and storage

Handling	Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on
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clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance.

Storage.

Keep containers tightly closed in a dry, cool and well-ventilated place. To maintain product quality: Keep refrigerated. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Isophoronediiisocyanate	TWA: 0.005 ppm	(Vacated) TWA: 0.005 ppm (Vacated) STEL: 0.02 ppm Skin	REL = 0.005 ppm (TWA) REL = 0.045 mg/m ³ (TWA) STEL: 0.02 ppm STEL: 0.180 mg/m ³	TWA: 0.005 ppm

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment**Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended Filter type:

Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-60 °C / -76 °F
Boiling Point/Range	153 °C / 307.4 °F @ 10 mmHg
Flash Point	163 °C / 325.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	4.5 vol %
Lower	0.7 vol %
Vapor Pressure	0.02 hPa @ 50°C
Vapor Density	No information available
Specific Gravity	1.061
Solubility	Insoluble in water
Partition coefficient; n-octanol/water	No data available

Autoignition Temperature	430 °C / 806 °F
Decomposition Temperature	> 260°C
Viscosity	13-15 mPa.sec @ 23°C
Molecular Formula	C12 H18 N2 O2
Molecular Weight	222.28

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Moisture sensitive.
Conditions to Avoid	Incompatible products. Excess heat. Exposure to moist air or water.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Nitrogen oxides (NO _x)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isophoronediiisocyanate	4814 mg/kg (Rat)	> 7000 mg/kg (Rat)	0.135 mg/L (Rat) 4 h

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	Irritating to eyes, respiratory system and skin
Sensitization	May cause sensitization by skin contact
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Isophoronediiisocyanate	4098-71-9	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects	No information available
Reproductive Effects	No information available.
Developmental Effects	No information available.
Teratogenicity	No information available.
STOT - single exposure	Respiratory system
STOT - repeated exposure	None known
Aspiration hazard	No information available
Symptoms / effects, both acute and delayed	Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
Endocrine Disruptor Information	No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Isophoronediiisocyanate	EC50: 118.7 mg/L/72h	Leuciscus idus: LC50: 1.8 mg/L/48h	Not listed	EC50:83.7 mg/L/24h

Persistence and Degradability based on information available. May persist

Bioaccumulation/ Accumulation No information available.

Mobility Is not likely mobile in the environment due its low water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No UN2290
Proper Shipping Name ISOPHORONE DIISOCYANATE
Hazard Class 6.1
Packing Group III

TDG

UN-No UN2290
Proper Shipping Name ISOPHORONE DIISOCYANATE
Hazard Class 6.1
Packing Group III

IATA

UN-No UN2290
Proper Shipping Name Isophorone diisocyanate
Hazard Class 6.1
Packing Group III

IMDG/IMO

UN-No UN2290
Proper Shipping Name Isophorone diisocyanate
Hazard Class 6.1
Packing Group III

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Isophoronediiisocyanate	4098-71-9	X	ACTIVE	-

Legend:

TSCA - US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export

Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Isophoronediiisocyanate	4098-71-9	X	-	223-861-6	X	X	X	X	X	KE-21479

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. 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.

Component	CAS No	Weight %	SARA 313 - Threshold Values %	SARA 313 - Reporting thresholds
Isophoronediiisocyanate	4098-71-9	<=100	1.0 %	-

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

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) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355).

Component	Hazardous Substances RQs	CERCLA Extremely Hazardous Substances RQs	SARA Reportable Quantity (RQ)
Isophoronediiisocyanate	-	500 lb	-

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Isophoronediiisocyanate	X	X	X	X	X

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security

This product does not contain any DHS chemicals.

Other International Regulations**Mexico - Grade**

Slight risk, Grade 1

Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isophoronediiisocyanate	4098-71-9	-	Use restricted. See entry 75. (see link for restriction details) Use restricted. See entry 74. (see link for restriction details)	-

REACH links<https://echa.europa.eu/substances-restricted-under-reach>**Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Isophoronediiisocyanate	4098-71-9	Listed	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Isophoronediiisocyanate	4098-71-9	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information**Prepared By**Health, Safety and Environmental Department
Email: chem.techinfo@thermofisher.com
www.thermofisher.com**Creation Date**

03-Sep-2009

Revision Date

29-Jul-2024

Print Date

29-Jul-2024

Revision Summary

Initial Release.

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 SDS