

## SAFETY DATA SHEET

Creation Date 03-September-2009

Revision Date 29-July-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

##### **Importer/Distributor**

Fisher Scientific  
112 Colonnade Road,  
Ottawa, ON K2E 7L6,  
Canada  
Tel: 1-800-234-7437

##### **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

##### **WHMIS 2015 Classification**

Classified as hazardous under the Hazardous Products Regulations (SOR/2015-17)

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

#### Label Elements

##### **Signal Word**

Danger

##### **Hazard Statements**

Fatal if inhaled  
Causes skin irritation  
May cause an allergic skin reaction  
Causes serious eye irritation  
May cause allergy or asthma symptoms or breathing difficulties if inhaled  
May cause respiratory irritation

**Precautionary Statements****Prevention**

Do not breathe dust/fumes/gas/mist/vapours/spray  
Wash face, hands and any exposed skin thoroughly after handling  
Use only outdoors or in a well-ventilated area  
Contaminated work clothing should not be allowed out of the workplace  
Wear protective gloves/protective clothing/eye protection/face protection  
Wear respiratory protection

**Response**

IF ON SKIN: Wash with plenty of soap and water  
IF INHALED: Remove person to fresh air and keep comfortable for breathing  
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/doctor  
Take off contaminated clothing and wash it before reuse

**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

**Other Hazards**

Toxic to aquatic life with long lasting effects

### 3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Isophorone diisocyanate	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/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<sub>2</sub>), 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 (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</sub>).

### 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 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	Alberta	British Columbia	Ontario TWA/EV	Quebec	ACGIH TLV	OSHA PEL	NIOSH
Isophorone diisocyanate	TWA: 0.005 ppm TWA: 0.05 mg/m <sup>3</sup>	TWA: 0.005 ppm Ceiling: 0.01 ppm	TWA: 0.005 ppm CEV: 0.02 ppm	TWA: 0.005 ppm TWA: 0.045 mg/m <sup>3</sup>	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 <sup>3</sup> (TWA) STEL: 0.02 ppm STEL: 0.180 mg/m <sup>3</sup>

#### 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.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

### Personal protective equipment

#### Eye Protection

Goggles

#### Hand Protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Glove material	Breakthrough time	Glove thickness	Glove comments
Nitrile rubber Neoprene Natural rubber PVC	See manufacturers recommendations	-	Splash protection only

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

#### Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. 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.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

When RPE is used a face piece Fit Test should be conducted

### Environmental exposure controls

Prevent product from entering drains. Do not allow material to contaminate ground water system.

### Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

## 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	C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
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 <sub>2</sub> ), Nitrogen oxides (NO <sub>x</sub> )
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
Isophorone diisocyanate	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
Isophorone diisocyanate	4098-71-9	Not listed	Not listed	Not listed	Not listed	Not listed

<b>Mutagenic Effects</b>	No information available
<b>Reproductive Effects</b>	No information available.
<b>Developmental Effects</b>	No information available.
<b>Teratogenicity</b>	No information available.
<b>STOT - single exposure</b>	Respiratory system
<b>STOT - repeated exposure</b>	None known
<b>Aspiration hazard</b>	No information available
<b>Symptoms / effects, both acute and delayed</b>	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
<b>Endocrine Disruptor Information</b>	No information available
<b>Other Adverse Effects</b>	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
Isophorone diisocyanate	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

<b>UN-No</b>	UN2290
<b>Proper Shipping Name</b>	ISOPHORONE DIISOCYANATE
<b>Hazard Class</b>	6.1
<b>Packing Group</b>	III

### TDG

<b>UN-No</b>	UN2290
<b>Proper Shipping Name</b>	ISOPHORONE DIISOCYANATE
<b>Hazard Class</b>	6.1
<b>Packing Group</b>	III

### IATA

<b>UN-No</b>	UN2290
<b>Proper Shipping Name</b>	Isophorone diisocyanate
<b>Hazard Class</b>	6.1
<b>Packing Group</b>	III

### IMDG/IMO

<b>UN-No</b>	UN2290
<b>Proper Shipping Name</b>	Isophorone diisocyanate
<b>Hazard Class</b>	6.1

## Packing Group

III

## 15. Regulatory information

## International Inventories

Component	CAS-No	DSL	NDSL	TSCA	TSCA Inventory notification - Active-Inactive	EINECS	ELINCS	NLP
Isophorone diisocyanate	4098-71-9	X	-	X	ACTIVE	223-861-6	-	-

Component	CAS-No	IECSC	KECL	ENCS	ISHL	TCSI	AICS	NZIoC	PICCS
Isophorone diisocyanate	4098-71-9	X	KE-21479	X	X	X	X	X	X

## Legend:

X - Listed '-' - Not Listed

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

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

## Canada

SDS in compliance with provisions of information as set out in Canadian Standard - Part 4, Schedule 1 and 2 of the Hazardous Products Regulations (HPR) and meets the requirements of the HPR (Paragraph 13(1)(a) of the Hazardous Products Act (HPA)).

Component	Canada - National Pollutant Release Inventory (NPRI)	Canadian Environmental Protection Agency (CEPA) - List of Toxic Substances	Canada's Chemicals Management Plan (CEPA)
Isophorone diisocyanate	Part 1, Group A Substance		

## Legend

NPRI - National Pollutant Release Inventory

## Other International Regulations

## Authorisation/Restrictions according to EU REACH

Component	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)
Isophorone diisocyanate	-	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)
Isophorone diisocyanate	4098-71-9	Listed	Not applicable	Not applicable	Not applicable

Component	CAS-No	Seveso III Directive (2012/18/EC) - Qualifying Quantities	Seveso III Directive (2012/18/EC) - Qualifying Quantities	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)

		for Major Accident Notification	for Safety Report Requirements		
Isophorone diisocyanate	4098-71-9	Not applicable	Not applicable	Not applicable	Not applicable

## 16. Other information

**Prepared By**

Product Safety Department  
Email: chem.techinfo@thermofisher.com  
www.thermofisher.com

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**Revision Summary**

Initial Release.

**Disclaimer**

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**End of SDS**