

SAFETY DATA SHEET

Version 6.4
Revision Date 13.09.2021
Print Date 31.01.2022**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Isophorone diisocyanate

Product Number : 317624

Brand : Aldrich

Index-No. : 615-008-00-5

CAS-No. : 4098-71-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : MilliporeSigma Canada Ltd
2149 WINSTON PARK DRIVE
OAKVILLE ON L6H 6J8
CANADA

Telephone : +1 905 829-9500

Fax : +1 905 829-9292

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA)
+1-703-527-3887 CHEMTREC
(International)
24 Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with Hazardous Products Regulations (HPR) (SOR/2015-17)**

Acute toxicity, Inhalation (Category 1), H330
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Respiratory sensitization (Category 1), H334
Skin sensitization (Category 1), H317
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

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.
H402 Harmful to aquatic life.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P272 Contaminated work clothing should not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.
P284 Wear respiratory protection.
P302 + P352 IF ON SKIN: Wash with plenty of water.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P362 + P364 Take off contaminated clothing and wash it before reuse.
P391 Collect spillage.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : 5-Isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane
Formula : C₁₂H₁₈N₂O₂
Molecular weight : 222.28 g/mol
CAS-No. : 4098-71-9

Aldrich - 317624

Page 2 of 11

EC-No. : 223-861-6
 Index-No. : 615-008-00-5

Component	Classification	Concentration *
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate		
	Acute Tox. 1; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; Aquatic Acute 3; Aquatic Chronic 2; H330, H315, H319, H334, H317, H335, H402, H411 Concentration limits: >= 0.5 %: Resp. Sens. 1, H334; >= 0.5 %: Skin Sens. 1, H317;	<= 100 %
* Weight %		

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Foam Water

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Moisture sensitive.

Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4098-71-9	C	0.01 ppm	Canada. British Columbia OEL
Remarks	Substance that has the potential to produce sensitization, as confirmed by human or animal data			
		TWA	0.0050 ppm 0.05 mg/m ³	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
		TWA	0.0050 ppm	Canada. British Columbia OEL
	Substance that has the potential to produce sensitization, as confirmed by human or animal data			
		TWAEV	0.0050 ppm 0.045 mg/m ³	Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants
	A substance to which exposure must be reduced to a minimum in accordance with section 42 Sensitizer			
		TWA	0.0050 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Respiratory sensitization			
		TWA	0.005 ppm	Canada. Ontario OELs

		C	0.02 ppm	Canada. Ontario OELs
--	--	---	----------	----------------------

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 120 min

Material tested: Butoject® (KCL 898)

Body Protection

protective clothing

Respiratory protection

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|--|--|
| a) Appearance | Form: liquid
Color: light yellow |
| b) Odor | pungent |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/freezing point: -60 °C (-76 °F) - (ECHA) |
| f) Initial boiling point and boiling range | 158 - 159 °C 316 - 318 °F at 20 hPa - lit. |
| g) Flash point | 163 °C (325 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, | No data available |

gas)	
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	< 0.1 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	1.049 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	ca.0.015 g/l at 23 °C (73 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	log Pow: 0.99 at 23 °C (73 °F) - OECD Test Guideline 107 - Bioaccumulation is not expected.
p) Autoignition temperature	430 °C (806 °F) at 1,013 hPa
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Alcohols
amides
Amines
Oxidizing agents
Ammonia
alkali hydroxides
glycol
phenol
urea
Water
mercaptans

10.4 Conditions to avoid

Avoid moisture.

Strong heating.

10.5 Incompatible materials

Metals

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 4,814 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 0.04 mg/l

(OECD Test Guideline 403)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Acute toxicity estimate Inhalation - 4 h - 0.0051 mg/l

(Expert judgment)

LD50 Dermal - Rat - male and female - > 7,000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

(Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Causes sensitization.

May cause sensitization by skin contact.

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Chromosome aberration test in vitro

Species: Mouse

Application Route: inhalation (vapor)

Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: NQ9370000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish static test LC50 - *Cyprinus carpio* (Carp) - > 208 mg/l - 96.0 h
(Regulation (EC) No. 440/2008, Annex, C.1)

Toxicity to daphnia and other aquatic invertebrates static test EC50 - *Daphnia magna* (Water flea) - 27 mg/l - 48 h
(Regulation (EC) No. 440/2008, Annex, C.2)

Toxicity to algae static test NOEC - *Desmodesmus subspicatus* (green algae) - 4.4 mg/l - 72 h
(Regulation (EC) No. 440/2008, Annex, C.3)

static test EC50 - *Desmodesmus subspicatus* (green algae) - > 70 mg/l - 72 h
(Regulation (EC) No. 440/2008, Annex, C.3)

Toxicity to bacteria static test EC50 - activated sludge - 263 mg/l - 3 h
(OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 0 % - Not readily biodegradable.
(Regulation (EC) No. 440/2008, Annex, C.4-D)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

TDG

UN number: 2290 Class: 6.1 Packing group: III
Proper shipping name: ISOPHORONE DIISOCYANATE
Labels: 6.1
ERG Code: 156
Marine pollutant: no

IMDG

UN number: 2290 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: ISOPHORONE DIISOCYANATE
Marine pollutant : yes

IATA

UN number: 2290 Class: 6.1 Packing group: III
Proper shipping name: Isophorone diisocyanate

SECTION 15: Regulatory information

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

SECTION 16: Other information

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

