SAFETY DATA SHEET

Version 6.5
Revision Date 09/13/2021
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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 : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

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 29 CFR 1910 (OSHA HCS)

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 must 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 soap and 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	Take off contaminated clothing and wash 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	:	$C_{12}H_{18}N_2O_2$
Molecular weight	:	222.28 g/mol
CAS-No.	:	4098-71-9
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 %

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 (NOx)
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

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4098-71-9	TWA	0.0050 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Respiratory sensitization		
		TWA	0.0050 ppm	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		STEL	0.02 ppm	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		TWA	0.0050 ppm 0.045 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		ST	0.02 ppm 0.18 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		

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, gas)	No data available
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/cm3 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

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

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

DOT (US)

UN number: 2290 Class: 6.1 Packing group: III
Proper shipping name: Isophorone diisocyanate
Reportable Quantity (RQ):
Poison Inhalation Hazard: 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

SARA 302 Components

	CAS-No.	Revision Date
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4098-71-9	2008-11-03

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	4098-71-9	2008-11-03

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

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.

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