SAFETY DATA SHEET

Version 5.8
Revision Date 05/24/2016
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

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
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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 sensitisation (Category 1), H334
Skin sensitisation (Category 1), H317
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Acute aquatic toxicity (Category 3), H402
Chronic aquatic toxicity (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/ vapours/ 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/ protective clothing/ 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.

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
Registration number	:	01-2119490408-31-XXXX

Hazardous components

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; H315, H317, H319, H330, H334, H335, H402, H411	<= 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Moisture sensitive.
Storage class (TRGS 510): Non-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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components 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
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 110 min
Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Colour: colourless, yellow
b)	Odour	No data available
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	158 - 159 °C (316 - 318 °F) at 20 hPa (15 mmHg) - 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)	Vapour pressure	0.000635 hPa (0.000476 mmHg) at 20 °C (68 °F) - OECD Test Guideline 104
l)	Vapour density	No data available
m)	Relative density	1.049 g/cm3 at 25 °C (77 °F) - lit.
n)	Water solubility	ca.0.015 g/l at 23 °C (73 °F) - OECD Test Guideline 105
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	430 °C (806 °F) at 1,013 hPa (760 mmHg)
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	Not explosive
t)	Oxidizing properties	No data available

9.2 Other safety information
No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Avoid moisture.

10.5 Incompatible materials
Strong oxidizing agents, Strong acids, Alcohols

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)
Other decomposition products - No data available
In the event of fire: see section 5

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 - 31 mg/m3
(OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - > 7,000 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Irritating to skin. - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Irritating to eyes.
(OECD Test Guideline 405)

Respiratory or skin sensitisation
in vivo assay - Guinea pig
May cause sensitisation by skin contact.
(OECD Test Guideline 406)

in vivo assay - Guinea pig
May cause sensitisation by inhalation.

Germ cell mutagenicity
In vitro mammalian cell gene mutation test
Chinese hamster ovary cells
Result: negative

OECD Test Guideline 474
Mouse - male
Result: negative

Carcinogenicity

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

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

No component 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 identified as a carcinogen or potential carcinogen by OSHA.

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

Developmental Toxicity - Rat - Inhalation
No significant adverse effects were reported

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	static test LC50 - Danio rerio (zebra fish) - >= 72 mg/l - 96 h (Tested according to Directive 92/69/EEC.)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 27 mg/l - 48 h (Directive 67/548/EEC, Annex V, C.2.)
Toxicity to algae	static test EC50 - Desmodesmus subspicatus (green algae) - > 70 mg/l - 72 h (Tested according to Directive 92/69/EEC.)
Toxicity to bacteria	Respiration inhibition 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.

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
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

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

15. REGULATORY INFORMATION

SARA 302 Components
The following components are subject to reporting levels established by SARA Title III, Section 302:

	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

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

Pennsylvania Right To Know Components

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

New Jersey Right To Know Components

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

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Irrit.	Eye irritation
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.
Resp. Sens.	Respiratory sensitisation
Skin Irrit.	Skin irritation

HMIS Rating

Health hazard:	4
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	4
Fire Hazard:	1
Reactivity Hazard:	0

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.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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