

SAFETY DATA SHEET

1. PRODUCT

1.1 Product identifiers

Name: Isophorone

CAS-No.: 78-59-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Dermal (Category 4), H312


Eye irritation (Category 2A), H319

Carcinogenicity (Category 2), H351

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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	Warning
Hazard statement(s)	H302 + H312 Harmful if swallowed or in contact with skin H319 Causes serious eye irritation. H335 May cause respiratory irritation. H351 Suspected of causing cancer.
Precautionary statement(s)	P201 Obtain special instructions before use. P202 Do not handle until all safety precautions have been read and understood. P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray. P264 Wash skin thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P271 Use only outdoors or in a well-ventilated area. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth. P302 + P352 + P312 IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell. P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell. P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P308 + P313 IF exposed or concerned: Get medical advice/ attention. P337 + P313 If eye irritation persists: Get medical advice/ attention. P363 Wash contaminated clothing before reuse. 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

No data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms:	3,5,5-Trimethyl-2-cyclohexen-1-one
Formula:	C ₉ H ₁₄ O
Molecular weight:	138.21 g/mol
CAS-No.:	78-59-1
EC-No.:	201-126-0

Hazardous components

Component	Classification	Concentration
Isophorone	Acute Tox. 4; Eye Irrit. 2A; Carc. 2; STOT SE 3; H302 + H312, H319, H335, H351	<= 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. 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

4.2 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

Use personal protective equipment. 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.

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.

Storage class (TRGS 510): Combustible liquids

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
Isophorone	78-59-1	C	5.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Malaise Fatigue Confirmed animal carcinogen with unknown relevance to humans		
		TWA 4.000000 ppm 23.000000 mg/m3 USA. NIOSH Recommended Exposure Limits		
		TWA 25.000000 ppm 140.000000 mg/m3 USA. Occupational Exposure Limits (OSHA) -Table Z-1 Limits for Air Contaminants		
		The value in mg/m3 is approximate.		
		PEL	4 ppm 23 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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).
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Skin protection	<p>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.</p> <p>Full contact Material: butyl-rubber Minimum layer thickness: 0.3 mm Break through time: 480 min Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)</p> <p>Splash contact Material: Nature latex/chloroprene Minimum layer thickness: 0.6 mm Break through time: 50 min Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M) data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374</p> <p>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.</p>
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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Appearance	Form: liquid, clear Colour: light yellow
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: -8 °C (18 °F) - lit.
Initial boiling point and boiling range	213 - 214 °C (415 - 417 °F) - lit.
Flash point	96.0 °C (204.8 °F) - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 3.8 %(V) Lower explosion limit: 0.8 %(V)
Vapour pressure	1.3 hPa (1.0 mmHg) at 38.0 °C (100.4 °F) 0.3 hPa (0.2 mmHg) at 20.0 °C (68.0 °F)
Vapour density	No data available
Relative density	0.923 g/cm ³ at 25 °C (77 °F)
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Auto-ignition temperature	462.0 °C (863.6 °F)
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
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

No data available

10.5 Incompatible materials

Strong oxidizing agents, Strong acids, Strong bases

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

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 - 1,870 mg/kg LC50 Inhalation - Guinea pig - 8 h - 4600 ppm LD50 Dermal - Rabbit - 1,382 mg/kg No data available
Skin corrosion/irritation
Skin - Rabbit Result: Mild skin irritation - 24 h
Serious eye damage/eye irritation
Eyes - Rabbit Result: Eye irritation - 24 h
Respiratory or skin sensitisation
No data available
Germ cell mutagenicity
No data available
Carcinogenicity
This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification. Limited evidence of carcinogenicity in animal studies 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. 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 No data available
Specific target organ toxicity -single exposure
May cause respiratory irritation.
Specific target organ toxicity -repeated exposure
No data available
Aspiration hazard
No data available
Additional Information
RTECS: GW7700000 burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Central nervous system depression, narcosis Central nervous system -

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	NOEC - <i>Cyprinodon variegatus</i> (sheepshead minnow) - 170 mg/l - 96 h LC50 - <i>Pimephales promelas</i> (fathead minnow) - 145 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	LC50 - <i>Daphnia magna</i> (Water flea) - 120 mg/l - 48 h
Toxicity to algae	No data available
Toxicity to bacteria	No data available

12.2 Persistence and degradability

12.3 Bioaccumulative potential

Bioaccumulation	<i>Lepomis macrochirus</i> (Bluegill) - 14 d - 0.0924 mg/l Bioconcentration factor (BCF): 7
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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

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 3082 Class: 9 Packing group: III

Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Isophorone)

Reportable Quantity (RQ): 5000 lbs

Poison Inhalation Hazard: No

IMDG

Not dangerous goods

IATA

Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

Component	CAS-No.	Revision Date
Isophorone	78-59-1	1993-04-24

Pennsylvania Right To Know Components

Component	CAS-No.	Revision Date
Isophorone	78-59-1	1993-04-24

New Jersey Right To Know Components

Component	CAS-No.	Revision Date
Isophorone	78-59-1	1993-04-24

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.

16. OTHER INFORMATION

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

Acute Tox. Acute toxicity

Carc. Carcinogenicity

Eye Irrit. Eye irritation

H302 Harmful if swallowed.

H302 + H312 Harmful if swallowed or in contact with skin

H312 Harmful in contact with skin.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

HMIS Rating

Health hazard: 2

Chronic Health Hazard: *

Flammability: 1

Physical Hazard 0

NFPA Rating

Health hazard: 2

Fire Hazard: 1

Reactivity Hazard: 0
