

SAFETY DATA SHEET

Version 6.12
Revision Date 09/09/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Isophorone

Product Number : W355305

Brand : Aldrich

Index-No. : 606-012-00-8

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

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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, Oral (Category 4), H302

Acute toxicity, Dermal (Category 4), H312

Eye irritation (Category 2A), H319

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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 Statements

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 Statements

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

P261

Avoid breathing mist or vapors.

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 water. Call a POISON CENTER/ doctor 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

Lachrymator.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : 3,5,5-Trimethyl-2-cyclohexen-1-one

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Formula : C₉H₁₄O
 Molecular weight : 138.21 g/mol
 CAS-No. : 78-59-1
 EC-No. : 201-126-0
 Index-No. : 606-012-00-8

Component	Classification	Concentration
isophorone		
	Acute Tox. 4; Eye Irrit. 2A; Carc. 2; STOT SE 3; H302, H312, H319, H351, H335 Concentration limits: >= 10 %: STOT SE 3, H335;	<= 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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

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

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Nature of decomposition products not known.

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

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 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.

Storage class

Storage class (TRGS 510): 10: Combustible liquids

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
isophorone	78-59-1	C	5 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans		
		TWA	4 ppm 23 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	25 ppm 140 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	4 ppm 23 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

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 EN 16523-1 please

contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 120 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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, clear
Color: light yellow |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/ range: -8 °C (18 °F) - lit. |
| f) Initial boiling point and boiling range | 213 - 214 °C 415 - 417 °F - lit. |
| g) Flash point | 96.0 °C (204.8 °F) - closed cup |

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h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 3.8 %(V) Lower explosion limit: 0.8 %(V)
k) Vapor pressure	1.3 hPa at 38.0 °C (100.4 °F) 0.3 hPa at 20.0 °C(68.0 °F)
l) Vapor density	No data available
m) Density	0.923 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	14.5 g/l - completely soluble
o) Partition coefficient: n-octanol/water	log Pow: 1.67 at 20 °C (68 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	462.0 °C (863.6 °F)
q) Decomposition temperature	No data available
r) Viscosity	2.83 mm ² /s at 20 °C (68 °F) - OECD Test Guideline 114 -
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:
Oxidizing agents

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

Strong oxidizing agents

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 - 1,500 mg/kg

Remarks: (ECHA)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages: damage of respiratory tract

Inhalation: Irritating to respiratory system.

LC50 Inhalation - Rat - male - 4 h - 7 mg/l - aerosol

Remarks: (ECHA)

LD50 Dermal - Rabbit - male and female - 1,200 mg/kg

Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(Draize Test)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: (National Toxicology Program)

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Result: Positive results were obtained in some in vitro tests.

Remarks: (ECHA)

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: Chromosome aberration test in vitro

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Test system: Chinese hamster lung cells
Metabolic activation: with and without metabolic activation
Result: Positive results were obtained in some in vitro tests.
Remarks: (ECHA)
Test Type: sister chromatid exchange assay
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA)
Test Type: unscheduled DNA synthesis assay
Test system: rat hepatocytes
Metabolic activation: without metabolic activation
Result: negative
Remarks: (ECHA)

Species: *Drosophila melanogaster* (vinegar fly)

Application Route: Oral

Result: negative
Remarks: (ECHA)

Test Type: Micronucleus test
Species: Mouse

Application Route: Intraperitoneal

Result: negative
Remarks: (ECHA)

Test Type: Chromosome aberration test

Result: negative
Remarks: (National Toxicology Program)

Carcinogenicity

Suspected of causing cancer.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (isophorone)

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

Inhalation - May cause respiratory irritation. - Respiratory Tract

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male - Oral - 90 Days - NOAEL (No observed adverse effect level) - 102.5 mg/kg

Remarks: (ECHA)

RTECS: GW7700000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Central nervous system depression, narcosis

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

Systemic effects:

After absorption of toxic quantities:

Nausea
Vomiting
Dizziness
CNS disorders
drop in blood pressure
Headache
inebriation
narcosis

Causes impaired function of:

Lungs
Liver
Kidney

A lethal effect is possible after the uptake of large quantities.

Handle in accordance with good industrial hygiene and safety practice.

Central nervous system -

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 228 mg/l - 96 h Remarks: (ECHA)
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Toxicity to daphnia and other aquatic invertebrates	static test LC50 - Daphnia magna (Water flea) - 120 mg/l - 48 h (US-EPA)
Toxicity to algae	static test EC50 - Desmodesmus subspicatus (green algae) - 475 mg/l - 72 h Remarks: (ECHA)
Toxicity to bacteria	EC10 - Pseudomonas putida - 435 mg/l - 18 h Remarks: (External MSDS)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - 4.2 - 15.6 mg/l - 32 d (US-EPA)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 95 % - Readily biodegradable.
(Directive 67/548/EEC Annex V, C.4.A.)

12.3 Bioaccumulative potential

Bioaccumulation Lepomis macrochirus - 14 Days
at 16 °C(isophorone)

Bioconcentration factor (BCF): 1.1 - 1.8

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Discharge into the environment must be avoided.

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.

SECTION 14: Transport information**DOT (US)**

UN number: 3082 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s.
Reportable Quantity (RQ): 5000 lbs
Poison Inhalation Hazard: No

IMDG

Not dangerous goods

IATA

Not dangerous goods

Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information**CERCLA Reportable Quantity**

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
isophorone	78-59-1	5000	5000

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard

SARA 313 : 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.

US State Regulations**Massachusetts Right To Know**

isophorone 78-59-1

Pennsylvania Right To Know

isophorone 78-59-1

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

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Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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