

• SAFETY DATA SHEET

Version 8.12
Revision Date 11/06/2025
Print Date 07/27/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Isophorone

Product Number : I18709
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

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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Acute toxicity (Oral) : Category 4

Acute toxicity (Dermal) : Category 4

Eye irritation : Category 2A

Carcinogenicity : Category 2

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

Other hazards

None known.

GHS label elements

Hazard pictograms :



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 : **Prevention:**
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P261 Avoid breathing mist or vapours.
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.
Response:
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.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 78-59-1

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
isophorone	78-59-1*	$\geq 90 - \leq 100$	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this 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.

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

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Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.
	Vapours 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.
Hazardous combustion products	: Nature of decomposition products not known.
Specific extinguishing methods	: No data available
Further information	: Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
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- Environmental precautions : Do not let product enter drains.
- 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Advice on safe handling : Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
- Further information on storage conditions : Tightly closed.
- Storage class : 10, Combustible liquids
- Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
isophorone	78-59-1	C	5 ppm	ACGIH
		TWA	4 ppm 23 mg/m ³	NIOSH REL
		TWA	25 ppm 140 mg/m ³	OSHA Z-1

Engineering measures : No data available

Personal protective equipment

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.

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.

Hand protection

Material : butyl-rubber
Break through time : 480 min
Glove thickness : 0.7 mm
Protective index : Full contact
Manufacturer : Butoject® (KCL 898)

Material : Nitrile rubber
Break through time : 120 min
Glove thickness : 0.4 mm
Protective index : Splash contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Remarks : 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).

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

Skin and body protection : protective clothing

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

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid (68 °F / 20 °C, 1,013 hPa)

Color : light yellow

Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: 18 °F / -8 °C Method: lit.
Boiling point/boiling range	: 415 - 417 °F / 213 - 214 °C Method: lit.
Flash point	: 204.8 °F / 96.0 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Self-ignition	: 863.6 °F / 462.0 °C
Upper explosion limit / Upper flammability limit	: 3.8 %(V)
Lower explosion limit / Lower flammability limit	: 0.8 %(V)
Vapor pressure	: 1.3 hPa (100.4 °F / 38.0 °C) 0.3 hPa (68.0 °F / 20.0 °C)
Relative vapour density	: No data available
Relative density	: No data available
Density	: 0.923 g/cm ³ (77 °F / 25 °C) Method: lit.
Solubility(ies) Water solubility	: 14.5 g/l completely soluble
Partition coefficient: n- octanol/water	: log Pow: 1.67 (68 °F / 20 °C) Bioaccumulation is not expected.
Autoignition temperature	: 864 °F / 462 °C
Decomposition	: No data available

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temperature

Viscosity

Viscosity, dynamic : No data available

Viscosity, kinematic : 2.83 mm²/s (68 °F / 20 °C)
Method: OECD Test Guideline 114
GLP: yes

Flow time : No data available

Explosive properties : No data available

Oxidizing properties : none

Molecular weight : 138.21 g/mol

Particle characteristics

Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

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.

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

Possibility of hazardous reactions : Violent reactions possible with:
Oxidizing agents

Conditions to avoid : Strong heating.

Incompatible materials : Strong oxidizing agents

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

Maximisation 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

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 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 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 - 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

Ecotoxicity

Components:

isophorone:

Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 228 mg/l
End point: mortality
Exposure time: 96 h
Test Type: flow-through test
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates : LC50 (Daphnia magna (Water flea)): 120 mg/l
End point: mortality
Exposure time: 48 h
Test Type: static test
Method: US-EPA

Toxicity to algae/aquatic : EC50 (Desmodesmus subspicatus (green algae)): 475

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plants	mg/l Exposure time: 72 h Test Type: static test Remarks: (ECHA)
Toxicity to fish (Chronic toxicity)	: NOEC (Pimephales promelas (fathead minnow)): 4.2 - 15.6 mg/l Exposure time: 32 d Test Type: flow-through test Analytical monitoring: yes Method: US-EPA
Toxicity to microorganisms	: EC10 (Pseudomonas putida): 435 mg/l Exposure time: 18 h Remarks: (External MSDS)

Persistence and degradability

Components:

isophorone:

Biodegradability	: aerobic Inoculum: activated sludge Concentration: 10 mg/l Result: Readily biodegradable. Biodegradation: 95 % Exposure time: 28 d Method: Directive 67/548/EEC Annex V, C.4.A. GLP: yes
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Bioaccumulative potential

Components:

isophorone:

Bioaccumulation	: Species: Lepomis macrochirus Bioconcentration factor (BCF): 1.1 - 1.8 Exposure time: 14 Days Temperature: 61 °F / 16 °C
Partition coefficient: n-octanol/water	: log Pow: 1.67 (68 °F / 20 °C) Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Components:

isophorone:

Additional ecological information	: Discharge into the environment must be avoided.
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SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 3082
Proper shipping name : Environmentally hazardous substance, liquid, n.o.s. (isophorone)
Class : 9
Packing group : III
Labels : Class 9 - Miscellaneous dangerous substances and articles
ERG Code : 171
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component	Calculated product
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		RQ (lbs)	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

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components 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

Full text of other abbreviations

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
 NIOSH REL : USA. NIOSH Recommended Exposure Limits
 OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
 ACGIH / C : Ceiling limit
 NIOSH REL / TWA : Time-weighted average concentration for up to a 10-

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

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hour workday during a 40-hour workweek
OSHA Z-1 / TWA : 8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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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Revision Date : 11/06/2025

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