Isophorone SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Isophorone
* Catalog Number: S2998
* CAS Number: 78-59-1
* IUPAC Name: 2-Cyclohexen-1-one, 3,5,5-trimethyl-

Relevant identified uses and uses advised against

* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

* Company: Selleck Chemicals
* TollFree: +1 877 796-6397
* Tel: +1 832 582-8158
* Fax: +1 832 582-8590

Emergency telephone number

* Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Flammable liquids: Category 4. H227
Acute toxicity (oral): Category 4. H302
Acute toxicity (dermal): Category 4. H312
Skin irritation: Category 3. H316
Serious eye irritation: Category 2. H319
Eye irritation: Category 2. H320
Acute toxicity (inhalation): Category 5. H333
Specific target organ toxicity (single exposure): Category 3. H335
Specific target organ toxicity (single exposure): Category 3. H336
Carcinogenicity: Category 2. H351

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word Warning

Hazard statement(s)	H227: Combustible liquid H302: Harmful if swallowed H312: Harmful in contact with skin H316: Causes mild skin irritation H319: Causes serious eye irritation H320: Causes eye irritation H333: May be harmful if inhaled H335: May cause respiratory irritation H336: May cause drowsiness or dizziness H351: Suspected of causing cancer
Precautionary statement(s)	None.
Prevention	P203: Obtain, read and follow all safety instructions before use. P210: Keep away from heat, hot surface, sparks, open flames and other ignition sources. No smoking. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. 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/hearing protection.
Response	P301+P317: IF SWALLOWED: Get medical help. P302+P352: IF ON SKIN: wash with plenty of water. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P317: Get emergency medical help. P318: if exposed or concerned, get medical advice. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P332+P317: If skin irritation occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P362+P364: Take off contaminated clothing and wash it before reuse. P370+P378: In case of fire: Use water spray, dry chemical, carbon dioxide, or appropriate foam to extinguish.
Storage	P403: Store in a well-ventilated place. P403+P233: Store in a well-ventilated place. Keep container tightly closed. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Isophorone

CAS Number: 78-59-1

PubChem CID: 6544

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

Skin contact: Remove contaminated clothes. Rinse and then wash skin with water and soap.

Eye contact: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion: Rinse mouth. Give a slurry of activated charcoal in water to drink. Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO2), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

CAUTION: The majority of these products have a very low flash point. Use of water spray when fighting fire may be inefficient. CAUTION: For mixtures containing alcohol or polar solvent, alcohol-resistant foam may be more effective.

SMALL FIRE: Dry chemical, CO2, water spray or regular foam. If regular foam is ineffective or unavailable, use alcohol-resistant foam.

LARGE FIRE: Water spray, fog or regular foam. If regular foam is ineffective or unavailable, use alcohol-resistant foam. Avoid aiming straight or solid streams directly onto the product. If it can be done safely, move undamaged containers away from the area around the fire.

FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. For petroleum crude oil, do not spray water directly into a breached tank car. This can lead to a dangerous boil over. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2024)

Use water spray, powder, foam, carbon dioxide.

Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use "alcohol" foam, dry chemical or carbon dioxide.

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped or safely confined. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use "alcohol" foam, dry chemical or carbon dioxide.

Use water spray to keep fire exposed containers cool. Use flooding quantities of water as fog or spray, dry chemical, foam, or carbon dioxide.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

Flash point: 184 °F (NTP, 1992)

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area for at least 50 meters (150 feet) in all directions.

LARGE SPILL: Consider initial downwind evacuation for at least 300 meters (1000 feet).

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

If leak or spill has not ignited, use water spray to disperse vapors & to protect men attempting to stop leak.

Environmental considerations: Land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner./ Dike surfact flow using soil, sand bags, foamed polyurethane, or foamed concrete. Absorb bulk liquid with fly ash, cement powder, or comercial sorbents.

Environmental considerations: Water spill: Use natural barriers or oil spill control booms to limit spill travel. Remove trapped material with suction hoses.

Environmental considerations: Air spill: Apply water spray or mist ot knock kown vapors.

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

The following wastewater treatment technologies have been investigated for Isophorone. Concentration process: Biological treatment.

The following wastewater treatment technologies have been investigated for Isophorone. Concentration process: Solvent extraction.

The following wastewater treatment technologies have been investigated for Isophorone. Concentration process: Activated carbon.

Spray into incinerator or burn in paper packaging. Additional flammable solvent may be added.

Irrigate eyes with water. Wash skin with abundant quantities of water.

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

SRP: Contaminated protective clothing should be segregated in such a manner so that there is no direct personal contact by personnel who handle, dispose, or clean the clothing. Quality assurance to ascertain the completeness of the cleaning procedures should be implemented before the decontaminated protective clothing is returned for reuse by the workers. Contaminated clothing should not be taken home at end of shift, but should remain at employee's place of work for cleaning.

Personnel protection: Avoid breathing vapors. Keep upwind. ... Do not handle broken packages unless wearing appropriate personal protective equipment. Wash away any material which may have contacted the body with copious amounts of water or soap and water.

For more Preventive Measures (Complete) data for ISOPHORONE (7 total), please visit the HSDB record page.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. All equipment used when handling the product must be grounded. Do not touch or walk through spilled material. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. A vapor-suppressing foam may be used to reduce vapors. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. Use clean, non-sparking tools to collect absorbed material.

LARGE SPILL: Dike far ahead of liquid spill for later disposal. Water spray may reduce vapor, but may not prevent ignition in closed spaces. (ERG, 2024)

Separated from strong oxidants, strong bases and amines.

store in a cool, dry, well-ventilated location. Outside or detached storage is preferred. Separate from oxidizing materials.

7.2 Conditions for safe storage, including any incompatibilities

Separated from strong oxidants, strong bases and amines.

store in a cool, dry, well-ventilated location. Outside or detached storage is preferred. Separate from oxidizing materials.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

Store in original container. Keep upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

11 mg/m

8.1.2 Appropriate engineering controls

Use only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Use NIOSH-approved dust/mist respirator (N95 or higher) if ventilation is inadequate.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Isophorone appears as a clear colorless liquid, with a camphor-like odor. Less dense than water and insoluble in water. Boiling point 420 °F. Flash point near 200 °F. Contact irritates skin and eyes. Toxic by ingestion. Used as a solvent and in pesticides.

b) Odor: Peppermint-like odor

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 18 °F (NTP, 1992)

f) Initial boiling point and boiling range: 419.4 °F at 760 mmHg (NTP, 1992)

g) Flash point: 184 °F (NTP, 1992)

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: 0.2 mmHg at 68 °F ; 1 mmHg at 100 °F (NTP, 1992)

l) Vapor density: No data available

m) Relative density: 0.921 at 77 °F (USCG, 1999) - Less dense than water; will float

n) Water solubility: 0.1 to 1 mg/mL at 64 °F (NTP, 1992)

o) Partition coefficient: n-octanol/water: Log P: No data available

p) Auto-ignition temperature: 864 °F (USCG, 1999)

q) Decomposition temperature: No data available

r) Viscosity: 2.62 cP @ 20 °C

s) Explosive properties: No data available

t) Oxidizing properties: No data available

9.2 Other information

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Incompatible with strong oxidizers

Oxidizers, strong alkalis, amines.

Oxidizers, strong alkalis, amines

10.6 Hazardous decomposition products

No data available.

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

Causes serious eye irritation (H319).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

Suspected of causing cancer (H351).

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

Carcinogen classification:

Isophorone

Group 2B: Possibly carcinogenic to humans

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Isophorone

TR-291: Toxicology and Carcinogenesis Studies of Isophorone (CASRN 78-59-1) in F344/N Rats and B6C3F1 Mice (Gavage Studies) (1986)

11/02/84

Some Evidence

No Evidence

Equivocal Evidence

No Evidence

Under the conditions of these 2-year gavage studies, there was some evidence of carcinogenicity of isophorone in male F344/N rats as shown by t

Exposure routes:

The substance can be absorbed into the body by inhalation, through the skin and by ingestion.

inhalation, ingestion, skin and/or eye contact

Signs and symptoms of exposure:

Burning sensation. Sore throat. Cough. Dizziness. Headache. Nausea. Shortness of breath.

Redness. Pain. Blurred vision.

Abdominal pain. Further see Inhalation.

irritation eyes, nose, throat; headache, nausea, dizziness, lassitude (weakness, exhaustion), malaise (vague feeling of discomfort), narcosis; dermatitis; In Animals: kidney, liver damage

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

LC50 Cyprinodon variegatus (sheepshead minnow) 166,000-295,000 ug/l/96 hr. /Conditions of bioassay not specified/

EC50 Selenastrum capricornutum (alga) 122,000 ug/l/96 hr, Toxic Effect: cell number reduced. /Conditions of bioassay not specified/

EC50 Selenastrum capricornutum (alga) 126,000 ug/l/96 hr, Toxic Effect: Chlorophyll a synthesis inhibited. /Conditions of bioassay not specified/

EC50 Skeletonema costatum (alga) 105,000 ug/l/96 hr, Toxic Effect: cell number reduced. /Conditions of bioassay not specified/

For more Ecotoxicity Values (Complete) data for ISOPHORONE (9 total), please visit the HSDB record page.

5.70e+02
2.40e+03
2.10e+03
8.80e+03
7.80e+01
5.00e+01
2.60e-02
9.50e-04
2.00e-01
2.00e+00
Volatile
Mutagen
1
0.1
3.80e+04
2.40e+05
6.30e+03
2.60e+04
7.80e+03
5.00e+01
9.50e-04
2.00e-01
2.00e+00
Volatile
Mutagen
1
0.1

Isophorone's production and use as a solvent for printing inks, lacquers, adhesives, and use as a chemical intermediate may result in its release to the environment through various waste streams. If released to air, a vapor pressure of 0.438 mm Hg at 25 °C indicates isophorone will exist solely as a vapor in the ambient atmosphere. Vapor-phase isophorone will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 5 hrs. If released to soil, isophorone is expected to have moderate mobility based upon an estimated Koc of 200. Volatilization from moist soil surf

12.2 Persistence and degradability

No data available.

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.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION

14.1 UN number

UN 1993

14.2 UN proper shipping name

Consult official transport regulations (DOT/IATA/IMDG) for proper shipping name.

14.3 Transport hazard class(es)

Consult official transport regulations (DOT/IATA/IMDG) for hazard classification.

DOT label: Combustible Liquid

14.4 Packing group

Consult official transport regulations (DOT/IATA/IMDG) for packing group assignment.

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

DOT Emergency Response Guide (ERG) number: 128

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

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 (short-term) health hazard

Chronic (long-term) health hazard

Fire hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

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

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: 2-Cyclohexen-1-one, 3,5,5-trimethyl-

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Carcinogenicity; Dermatotoxicity; Developmental Toxicity; Hepatotoxicity and Digestive System Toxicity; Neurotoxicity; Respiratory Toxicity Authoritative List - CA TACs; CWA 303(c); CW

- EFSA Legal Basis: Regulation (EC) No 1831/2003 (amended)

- New Jersey Worker and Community Right to Know Act: The New Jersey Worker and Community Right to Know Act requires public and private employers to provide information about hazardous substances at their workplaces. (N.J.S.A. 34:5A-1 et. seq.)

- Atmospheric Standards: This action promulgates standards of performance for equipment leaks of Volatile Organic Compounds (VOC) in the Synthetic Organic Chemical Manufacturing Industry (SOCMI). The intended effect of these standards is to require all newly constructed, modified, and reconstructed SOCMI process units to us

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.