

Section 1. Product and Company Identification

**Product Name** Isophorone  
**CAS Number** 78-59-1

**Parchem - fine & specialty chemicals**  
**415 Huguenot Street**  
**New Rochelle, NY 10801**  
☎ (914) 654-6800 ☎ (914) 654-6899  
🌐 [parchem.com](http://parchem.com) ✉ [info@parchem.com](mailto:info@parchem.com)

EMERGENCY RESPONSE NUMBER  
CHEMTEL  
Toll Free US & Canada: 1 (800) 255-3924  
All other Origins: 1 (813) 248-0585  
Collect Calls Accepted

Section 2. Hazards Identification

**Classification of the substance or mixture**

**Classification (GHS-US)**

Flam. Liq. 4, H227  
Acute Tox. 4 (Oral), H302  
Acute Tox. 4 (Dermal), H312  
Eye Irrit. 2A, H319  
Carc. 2, H351  
STOT SE 3, H335

**GHS Label Elements**

**Pictograms:**



**Signal word:** WARNING

**Hazard and precautionary statements**

**Hazard statements (GHS-US)**

H227 - Combustible liquid  
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 (GHS-US)**

P201 - Obtain special instructions before use  
P202 - Do not handle until all safety precautions have been read and understood  
P210 - Keep away from heat, hot surfaces, open flames, sparks. - No smoking



- P261 - Avoid breathing dust, fume, gas, mist, spray, vapors
- P264 - Wash hands 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 eye protection, protective clothing, protective gloves
- P301+P312 - If swallowed: Call a doctor, a POISON CENTER if you feel unwell
- 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+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
- P312 - Call a doctor, a POISON CENTER if you feel unwell
- P321 - Specific treatment (see a doctor on this label)
- P330 - Rinse mouth
- P337+P313 - If eye irritation persists: Get medical advice/attention
- P362+P364 - Take off contaminated clothing and wash it before reuse
- P370+P378 - In case of fire: Use alcohol resistant foam, carbon dioxide (CO<sub>2</sub>), dry extinguishing powder, Water spray to extinguish
- P403+P233 - Store in a well-ventilated place. Keep container tightly closed
- P403+P235 - Store in a well-ventilated place. Keep cool
- P405 - Store locked up
- P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

Section 3. Composition / Information on Ingredients

<b>Common Name</b>	Isophorone
<b>Synonym(s)</b>	2-Cyclohexen-1-one, 3,5,5-trimethyl-; 3,5,5-Trimethylcyclohex-2-en-1-one
<b>Formula</b>	C <sub>9</sub> H <sub>14</sub> O
<b>CAS Number</b>	78-59-1

COMPONENT	CAS NUMBER	CONCENTRATION
Isophorone	78-59-1	≥ 99%

Section 4. First Aid Measures

**Description of first-aid measures**

**Inhalation:** Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician if you feel unwell.

**Skin contact:** Remove affected clothing and wash all exposed skin area with mild soap and water, followed by warm water rinse. Immediately call a poison center or doctor/physician. Specific measures (see Consult a doctor/medical service on this label). Wash with plenty of soap and water. Wash contaminated clothing before reuse.



**Eye contact:** Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Consult an eye specialist. Get medical advice/attention.

**Ingestion:** Rinse mouth. Do NOT induce vomiting. Obtain emergency medical attention. Call a POISON CENTER or doctor/physician if you feel unwell.

### Most important symptoms and effects, both acute and delayed

**Inhalation:** May cause respiratory irritation.

**Skin contact:** Repeated exposure to this material can result in absorption through skin causing significant health hazard.

**Eye contact:** Causes serious eye irritation.

**Ingestion:** Swallowing a small quantity of this material will result in serious health hazard.

**Indication of any immediate medical attention and special treatment needed:** No additional information available

## Section 5. Firefighting Measures

### Extinguishing media

**Suitable extinguishing media:** Foam. Dry powder. Carbon dioxide. Water spray. Sand.

**Unsuitable extinguishing media:** Do not use a heavy water stream.

### Special hazards arising from the substance or mixture

**Fire hazard:** Combustible liquid.

**Explosion hazard:** May form flammable/explosive vapor-air mixture.

### Advice for firefighters

**Firefighting instructions:** Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire. Prevent fire-fighting water from entering environment.

**Protection during firefighting:** Do not enter fire area without proper protective equipment, including respiratory protection.

## Section 6. Accidental Release Measures

### Personal precautions, protective equipment and emergency procedures

**General measures:** Remove ignition sources. Use special care to avoid static electric charges. No open flames. No smoking.

### For non-emergency personnel

**Emergency procedures:** Evacuate unnecessary personnel.

### For emergency responders

**Protective equipment:** Equip cleanup crew with proper protection.

**Emergency procedures:** Ventilate area.



**Environmental precautions:** Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

**Methods and material for containment and cleaning up**

**Methods for cleaning up:** Soak up spills with inert solids, such as clay or diatomaceous earth as soon as possible. Collect spillage. Store away from other materials.

**Reference to other sections:** See Heading 8. Exposure controls and personal protection.

Section 7. Handling and Storage

**Precautions for safe handling**

**Additional hazards when processed:** Handle empty containers with care because residual vapors are flammable. Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

**Precautions for safe handling:** Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Provide good ventilation in process area to prevent formation of vapor. No open flames. No smoking. Obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Avoid breathing dust, fume, gas, mist, vapors, spray. Use only outdoors or in a well-ventilated area.

**Hygiene measures:** Do not eat, drink or smoke when using this product. Wash hands thoroughly after handling.

**Conditions for safe storage, including any incompatibilities**

**Technical measures:** Proper grounding procedures to avoid static electricity should be followed.

**Storage conditions:** Keep only in the original container in a cool, well ventilated place away from: Ignition sources or incompatible materials. Keep in fireproof place. Keep container tightly closed.

**Incompatible products:** Strong bases. Strong acids.

**Incompatible materials:** Sources of ignition. Direct sunlight. Heat sources.

Section 8. Exposure Controls / Personal Protection

**Control parameters**

<b>Isophorone (78-59-1)</b>		
ACGIH	ACGIH Ceiling (ppm)	5 ppm
ACGIH	Remark (ACGIH)	Eye & URT irr; CNS impair;
OSHA	OSHA PEL (TWA) (mg/m <sup>3</sup> )	140 mg/m <sup>3</sup>
OSHA	OSHA PEL (TWA) (ppm)	25 ppm

**Personal protective equipment:** Avoid all unnecessary exposure.

**Hand protection:** Wear protective gloves.

**Eye protection:** Chemical goggles or safety glasses.

**Respiratory protection:** Wear appropriate mask.

**Other information:** Do not eat, drink or smoke during use.

Section 9. Physical and Chemical Properties

**Physical state:** Liquid

**Appearance:** Colorless liquid.

**Color:** Colorless

**Odor:** peppermint-like camphor-like

**Odor threshold**

0.19 ppm (Hellman and Small)

1.1 mg/m<sup>3</sup> (Hellman and Small)

**pH:** No data available

**Melting point:** -8.1°C ; 17.6°F

**Freezing point:** No data available

**Boiling point:** 215°C ; 419.0°F

**Flash point:** 84°C ; 183.2°F Closed cup

**Relative evaporation rate (butyl acetate=1):** No data available

**Flammability (solid, gas):** No data available

**Explosion limits:** 0.8 - 3.8 vol %

**Explosive properties:** No data available

**Oxidizing properties:** No data available

**Vapor pressure:** 0.4 hPa (at 20°C)

**Relative density:** 0.92

**Relative vapor density at 20°C:** 4.8

**Specific gravity/density:** 0.92 g/cm<sup>3</sup> (at 20°C)

**Molecular mass:** 138.2 g/mol

**Solubility:** Water: 12 g/l (at 20°C)

**Log Pow:** 1.66 (at 23°C)

**Log Kow:** No data available

**Auto-ignition temperature:** 460°C; 860.0°F

**Decomposition temperature:** No data available

**Viscosity:** No data available

**Viscosity, kinematic:** No data available

**Viscosity, dynamic:** No data available

**Other information**

No additional information available

Section 10. Stability and Reactivity

**Reactivity:** No additional information available

**Chemical stability:** Combustible liquid. May form flammable/explosive vapor-air mixture.

**Possibility of hazardous reactions:** Not established.



**Conditions to avoid:** Direct sunlight. Extremely high or low temperatures. Open flame. Overheating. Heat. Sparks.

**Incompatible materials:** Strong acids. Strong bases.

**Hazardous decomposition products:** fume. Carbon monoxide. Carbon dioxide. May release flammable gases.

Section 11. Toxicological Information

**Information on toxicological effects**

**Acute toxicity**

**Oral:** Harmful if swallowed.

**Dermal:** Harmful in contact with skin.

**Isophorone (78-59-1)**

LD50 oral rat	1870 mg/kg
LD50 dermal rat	1700 mg/kg
LC50 inhalation rat (mg/l)	7 mg/l/4h
ATE US (oral)	1870.000 mg/kg body weight
ATE US (dermal)	1700.000 mg/kg body weight
ATE US (vapors)	7.000 mg/l/4h
ATE US (dust, mist)	7.000 mg/l/4h

**Skin corrosion/irritation:** Not classified

**Serious eye damage/irritation:** Causes serious eye irritation.

**Respiratory or skin sensitization:** Not classified

**Germ cell mutagenicity:** Not classified

**Carcinogenicity:** Suspected of causing cancer.

**Isophorone (78-59-1)**

National Toxicology Program (NTP) Status 1 - Evidence of Carcinogenicity	
--	--

**Reproductive toxicity:** Not classified

**Specific target organ toxicity (single exposure):** May cause respiratory irritation.

**Specific target organ toxicity (repeated exposure):** Not classified

**Aspiration hazard:** Not classified

**Potential Adverse human health effects and symptoms:** Based on available data, the classification criteria are not met. Harmful if swallowed. Harmful in contact with skin.

**Symptoms/injuries after inhalation:** May cause respiratory irritation.

**Symptoms/injuries after skin contact:** Repeated exposure to this material can result in absorption through skin causing significant health hazard.

**Symptoms/injuries after eye contact:** Causes serious eye irritation.

**Symptoms/injuries after ingestion:** Swallowing a small quantity of this material will result in serious health hazard.



Section 12. Ecological Information

**Toxicity**

**Isophorone (78-59-1)**

LC50 fish 1	132 - 159 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
EC50 Daphnia 1	117 mg/l (Exposure time: 48 h - Species: Daphnia magna)
LC50 fish 2	180 - 250 mg/l (Exposure time: 96 h - Species: Lepomis macrochirus [static])

**Persistence and degradability**

**Isophorone (78-59-1)**

Persistence and degradability	Not established.
-------------------------------	------------------

**Bioaccumulative potential**

**Isophorone (78-59-1)**

BCF fish 1 7	
Log Pow	1.66 (at 23°C)
Bioaccumulative potential	Not established.

**Mobility in soil:** No additional information available

**Other adverse effects**

**Other information:** Avoid release to the environment.

Section 13. Disposal Considerations

**Waste Treatment Methods:** Dispose of product and contaminated packaging in accordance with all local, state, and federal environmental control regulations.

Section 14. Transport Information

**Department of Transportation (DOT)**

**In accordance with DOT**

**Transport document description:** NA1993 Combustible liquid, n.o.s. (Isophorone), 3, III

**UN-No.(DOT):** NA1993

**Proper Shipping Name (DOT):** Combustible liquid, n.o.s. Isophorone

**Transport hazard class (DOT):** 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120

**Packing group (DOT):** III - Minor Danger

**DOT Packaging Non Bulk (49 CFR 173.xxx):** 203



**DOT Packaging Bulk (49 CFR 173.xxx):** 241

**DOT Symbols:** D - Proper shipping name for domestic use only, or to and from Canada, G - Identifies PSN requiring a technical name

**DOT Special Provisions (49 CFR 172.102):** IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50°C (1.1 bar at 122 °F), or 130 kPa at 55°C (1.3 bar at 131°F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672).

T1 - 1.5 178.274(d)(2) Normal 178.275(d)(2)

T4 - 2.65 178.274(d)(2) Normal 178.275(d)(3)

TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling =  $97 / 1 + a (tr - tf)$  Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.

**DOT Packaging Exceptions (49 CFR 173.xxx):** 150

**DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27):** 60 L

**DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75):** 220 L

**DOT Vessel Stowage Location:** A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

**Additional information**

**Other information:** No supplementary information available.

**ADR:** No additional information available

**Transport by sea:** No additional information available

**Air transport:** No additional information available

Section 15. Regulatory Information

**US Federal regulations**

**Isophorone (78-59-1)**

Listed on the United States TSCA (Toxic Substances Control Act) inventory	
EPA TSCA Regulatory Flag	T - T - indicates a substance that is the subject of a Section 4 test rule under TSCA.
RQ (Reportable quantity, section 304 of EPA's List of Lists)	5000 lb

**International regulations**

**CANADA**

**Isophorone (78-59-1)**

Listed on the Canadian DSL (Domestic Substances List)	
WHMIS Classification	Class B Division 3 - Combustible Liquid Class D Division 2 Subdivision B - Toxic material causing other toxic effects





### EU-Regulations

#### Isophorone (78-59-1)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Not classified

### Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

Not classified

### National regulations

#### Isophorone (78-59-1)

Listed on the AICS (Australian Inventory of Chemical Substances)

Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)

Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory

Listed on the Korean ECL (Existing Chemicals List)

Listed on NZIoC (New Zealand Inventory of Chemicals)

Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

Listed on the Canadian IDL (Ingredient Disclosure List)

Listed on INSQ (Mexican national Inventory of Chemical Substances)

Listed on Turkish inventory of chemical

### US State regulations

#### Isophorone(78-59-1)

State or local regulations	U.S. - Massachusetts - Right To Know List
	U.S. - New Jersey - Right to Know Hazardous Substance List
	U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List
	U.S. - Pennsylvania - RTK (Right to Know) List

### Section 16. Other Information

**Disclaimer:** 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.

REVISION DATE: 7/16/2015