

Material Safety Data for: Isophorone

1. PRODUCT IDENTIFICATION

Name 3,5,5-trimethyl-2-hexene-1-one
Synonyms isophorone, 1,1,3-trimethyl-3-hexene-5-one, & others
CAS# 78-59-1
Product Uses high boiling solvent for resins, coatings, inks, plastics, waxes, fats, oils; organic synthesis

<u>2. INGREDIENTS</u>	%	TWAEV / TLV mg/m ³	LD ₅₀ ORAL	(mg/kg) SKIN	LC ₅₀ ppm INHALATION
3,5,5-trimethyl-2-hexene-1-one	100%	5 / 28	1870	700	815

3. (a) HAZARDS SUMMARY

Hazards, Quick Guide: combustible liquid, may irritate skin & eyes, central nervous depressant, animal carcinogen

Canada – WHMIS
Key:

B 3, D 2B
B 2 – Flash Point <38°C, B 3 – Flash Point >38°C & <93°C
D 1 – Immediately Toxic, D 2 – Chronic Toxicity
C – Oxidising Substance, E – Corrosive

U.S.A. – HMIS
Key:

Health – 2, Fire – 2, Reactivity – 0
0=minimal, 1=slight, 2=moderate, 3=serious, 4=severe

3. (b) HAZARDS – TOXICITY

Effects, Acute Exposure

Skin Contact may irritate
 Skin Absorption slight; no toxic effects likely by this route
 Eye Contact severely irritating
 Inhalation 15-25ppm for 15 minutes or 40-80ppm for 1-2 minutes irritating; 200-400ppm* may causes headache, dizziness, drowsiness, nausea, intoxication
 Ingestion not known; likely to be irritating to mouth and throat – not a route of industrial exposure
**This high concentration is unlikely to occur in an industrial setting.*

Effects, Chronic Exposure

General no human information; animal tests suggest that >50ppm may damage lung & kidneys
 Sensitising not a sensitiser in humans or animals
 Carcinogen/Tumorigen renal tumors in ♂rats (*of a type not seen in ♀rats, or humans*); no known effect in humans
 Reproductive Effect no known effect in humans or animals
 Mutagen no known effect on humans or animals
 Synergistic With tetrachloroethylene, propylene oxide
 LD₅₀ (oral) 1870, 2000 & 2150mg/kg (rat), 2000 & 2690mg/kg (mouse), 1420mg/kg (rabbit), 700mg/kg (guinea pig)
 LD₅₀ (skin) 1390mg/kg (rat), 1380mg/kg (rabbit)
 LC₅₀ (inhalation) 1240ppm (rat), 815ppm** (guinea pig),
***600ppm is the maximum concentration of isophorone vapour @ 25°C. The above exposures must have been to vapour & mist combined, & may not be accurately measurable.*

Please ensure that this MSDS is given to, and explained to people using this product.

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4. FIRST AID

- SKIN:** Wash with soap and plenty of water. Remove contaminated clothing and do not reuse until thoroughly cleaned or laundered.
- EYES:** Wash eyes with plenty of water, holding eyelids open. Seek medical assistance promptly if there is irritation.
- INHALATION:** Remove from contaminated area promptly. **CAUTION: Rescuer must not endanger himself!** If breathing stops, administer artificial respiration and seek medical aid promptly.
- INGESTION:** Give plenty of water to dilute product. Do not induce vomiting (NOTE below). Keep victim quiet. If vomiting occurs, lower victim's head below hips to prevent inhalation of vomited material. Seek medical help promptly.

Inadvertent inhalation of vomited material may seriously damage the lungs. The danger of this is greater than the risk of poisoning through absorption of this relatively low-toxicity substance. The stomach should only be emptied under medical supervision, and after the installation of an airway to protect the lungs.

5. PHYSICAL PROPERTIES

Odour & Appearance	clear, colourless liquid with mild, pleasant, ethereal peppermint odour
Odour Threshold	~0.5ppm
Vapour Pressure	0.3mmHg / 0.04kPa (20°C / 68°F)
Evaporation Rate (<i>Butyl Acetate</i> = 1)	0.02
Vapour Density (air = 1)	4.8
Boiling Range	215°C / 419°F
Freezing Point	-8°C / 17°F
Specific Gravity	0.922 (20/20°C)
Water Solubility	12 grams per litre (20°C / 68°F)
Also soluble in	most organic solvents
Viscosity	2.6 centipoise (20°C / 68°F)
pH	none – (<i>does not liberate hydrogen ions when dissolved</i>)
Conversion Factor	1ppm = 5.64mg/m ³
Molecular Weight	138grams per mole

6. FLAMMABILITY & FIRE FIGHTING

Flash Point	84°C / 184°F (closed cup)
Autoignition Temperature	460°C / 860°F
Flammable Limits	0.8% – 3.8%
Combustion Products	carbon monoxide, nitrogen oxides, smoke, part oxidised hydrocarbon fragments
Fire Fighting Precautions	foam, dry chemical, water fog or spray, product floats on water – water jet spreads flames; fire fighters must wear SCBA
Static Charge Accumulation	probably cannot accumulate a static charge on agitation or pumping

7. STABILITY / REACTIVITY

Dangerously Reactive With	strong oxidising agents; strong acids or strong alkalies
Also Reactive With	reaction with amines may be vigorous
Stability	stable; will not polymerize
Decomposes in Presence of	not known
Decomposition Products	none apart from Hazardous Combustion Products
Sensitive to Mechanical Impact	no

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8. PROTECTIVE EQUIPMENT / EXPOSURE CONTROL

ACGIH TLV	5ppm / 28mg/m ³
OSHA PEL	25ppm / 140mg/m ³
STEL	not listed
Ventilation	mechanical ventilation is probably not required due to low vapour pressure
Hands	butyl rubber gloves – <i>other types may also protect; consult supplier to confirm suitability</i>
Eyes	safety glasses with side shields – <i>always protect the eyes</i>
Clothing	no special protective clothing required

9. HANDLING & STORAGE

Store in a cool, dry environment, away from sources of ignition, heat, oxidising agents and substances named in Part 8. Empty containers may contain a flammable / explosive vapour. Always ensure that containers, whether empty or full, or part full, are tightly sealed unless in use.

Avoid generating or breathing product mist. If mist is created in processing, install adequate ventilation. If dealing with a spill, and ventilation is impossible or impractical, wear a suitable respirator with organic vapour cartridge.

Never cut, drill, weld or grind on or near this container. Avoid prolonged contact with skin and wash work clothes frequently. An eye bath and safety shower must be available near the workplace.

10. SPILL PROCEDURES

Leak Precaution	dyke to control spillage and prevent environmental contamination
Handling Spill	ventilate contaminated area; recover free liquid with suitable pumps; absorb residue on an inert sorbent, sweep, shovel, & store in closed containers for recycling or disposal

11. DISPOSAL

Waste Disposal	do not flush to sewer , recycle solvent if possible, may be incinerated in approved facility; a flammable waste may be added to improve combustion
Containers	Drums should be reused. Recondition and pressure test by a licensed reconditioner prior to re-use. Pails must be vented and thoroughly dried prior to crushing and recycling. IBCs (intermediate bulk containers): polyethylene bottle must be pressure tested & recertified at 30 months. Replace at 60 months (5yrs). Steel containers must be inspected, pressure tested & recertified every 5 years. <i>Never cut, drill, weld or grind on or near this container, even if empty</i>

12. ENVIRONMENTAL INFORMATION

Bioaccumulation	this product is not a bioaccumulator
Biodegradation	this product may degrade slowly in the presence of oxygen; <i>some test procedures show rapid degradation, others suggest isophorone may resist degradation</i>
Abiotic Degradation	this product reacts with atmospheric hydroxyl radicals; estimated ½-life in air is 4 hours
Mobility in soil, water	this product is water soluble and will move readily in soil and water
Aquatic Toxicity	
LC ₅₀ (Fish, 96hr)	140 & 170mg/litre (Cyprinodon variegatus), 145, 228 & 255mg/litre (Pimephelas promelas), 224 & 240mg/litre (Lepomis macrochirus), & others
EC ₅₀ (Crustacea, 24hr)	430mg/litre (Artemia salina), 254 & 430mg/litre (Daphnia magna)
EC ₅₀ (Algae)	475mg/litre (Scenedesmus subspicatus, 72hr), 126mg/litre (Selenastrum capricornutum, 96hr)
EC ₅₀ (Bacteria)	100mg/litre (domestic sewage sludge), 420mg/litre (Tetrahymena pyriformis)

13. TRANSPORT REGULATIONS

Canada TDG	PIN	UN- not regulated for transport
	AND	Shipping Name not regulated for transport
U.S.A. 49 CFR	Class	not regulated for transport
	Packing Group	not regulated for transport
Marine Pollutant		not a marine pollutant

14. EMERGENCY INFORMATION

Canada	Call CANUTEC (collect)	(613) 996-6666
U.S.A.	Call CHEMTREC	(800) 424-9300

15. REGULATIONS

Canada DSL	on inventory
U.S.A. TSCA	on inventory
Europe EINECS	on inventory (EC# 201-126-0)

Immediately Dangerous to Life or Health: 200 ppm

Allowable Tolerances: Isophorone is exempted from the requirement of a tolerance when used as a solvent or cosolvent in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only.

OSHA Standards: Permissible Exposure Limit: Table Z-1 8-hr Time Weighted Avg: 25 ppm (140 mg/cu m).

NIOSH Recommendations: Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 4 ppm (23 mg/cu m).

Threshold Limit Values: Ceiling Limit: 5 ppm. A3; Confirmed animal carcinogen with unknown relevance to humans.

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 use the best demonstrated system of continuous emission reduction for equipment leaks of VOC, considering costs, non air quality health and environmental impact and energy requirements. Isophorone is produced, as an intermediate or a final product, by process units covered under this subpart. Listed as a hazardous air pollutant (HAP) generally known or suspected to cause serious health problems. The Clean Air Act, as amended in 1990, directs EPA to set standards requiring major sources to sharply reduce routine emissions of toxic pollutants. EPA is required to establish and phase in specific performance based standards for all air emission sources that emit one or more of the listed pollutants. Isophorone is included on this list.

Federal Drinking Water Guidelines: EPA 100 ug/l

State Drinking Water Guidelines: Florida 40 ug/l, Maine 370 ug/l, Minnesota 100 ug/l, New Hampshire 100 ug/l

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15. REGULATIONS, cont'd

Clean Water Act Requirements: Toxic pollutant designated pursuant to section 307(a)(1) of the Federal Water Pollution Control Act and is subject to effluent limitations.

CERCLA Reportable Quantities: Persons in charge of vessels or facilities are required to notify the National Response Center (NRC) immediately, when there is a release of this designated hazardous substance, in an amount equal to or greater than its reportable quantity of 5000 lb or 2270 kg. The toll free number of the NRC is (800) 424-8802; In the Washington D.C. metropolitan area (202) 426-2675. The rule for determining when notification is required is stated in 40 CFR 302.4 (section IV. D.3.b).

TSCA Requirements: Pursuant to section 8(d) of TSCA, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. Isophorone is included on this list. Section 8(a) of TSCA requires manufacturers of this chemical substance to report preliminary assessment information concerned with production, exposure, and use to EPA as cited in the preamble in 51 FR 41329.

FIFRA Requirements: Isophorone is exempted from the requirement of a tolerance when used as a solvent or cosolvent in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only.

FDA Requirements: Isophorone is listed as an indirect food additive for use only as a component of adhesives.

16. PREPARATION INFORMATION

Prepared for Megaloid Laboratories by Peter Bursztyn, (705) 734-1577

File Name: **Isophorone**

With data from RTECS, Haz. Substance Data Base, Cheminfo (CCOHS), IUCALID Datasheets (European Chem. Substance Info. System), & others, as available

*Preparation Date: **December 2006** Revision Date: **November 2009***

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