



Safety Data Sheet

1. PRODUCT IDENTIFICATION

Name	Isophorone
Synonyms	3,5,5-trimethyl-2-cyclohexene-1-one, 1,1,3-trimethyl-3-cyclohexene-5-one, & others
CAS#	78-59-1
Europe EC#	201-126-0
Product Uses	high boiling solvent for resins, coatings, inks, plastics, waxes, fats, oils; organic synthesis

2. 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, **F** – Reactive Substance



B3 – Combustible Liquid



D2B – Toxic

U.S.A. – HMIS

Key:

Health – 2, Fire – 2, Reactivity – 0

0=minimal, 1=slight, 2=moderate, 3=serious, 4=severe

3. COMPOSITION

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

4. FIRST AID

SKIN:	Wash with plenty of water. Remove contaminated clothing and do not reuse until thoroughly 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. FIRE FIGHTING & FLAMMABILITY

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
Firefighting Precautions	foam, dry chemical, water fog or spray, product floats on water – water jet spreads flames; firefighters must wear SCBA
Static Charge Accumulation	probably cannot accumulate a static charge on agitation or pumping

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

6. ACCIDENTAL RELEASE MEASURES

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

7. HANDLING & STORAGE

Store in a cool, dry environment, away from sources of ignition, heat, oxidising agents and substances named in Part 10. On prolonged storage, diacetone alcohol may break down to form highly flammable acetone. 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.

8. EXPOSURE CONTROL & PERSONAL PROTECTION

Ontario CEV	5ppm / 28mg/m ³
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 or polyvinyl alcohol gloves – <i>other types 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. 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=1</i>)	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

10. REACTIVITY

Dangerously Reactive With	strong oxidising agents; strong acids or strong alkalis
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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11. TOXICITY

Effects, Acute Exposure

Skin Contact	probably not irritating
Skin Absorption	slight; no toxic effects likely by this route
Eye Contact	severely irritating
Inhalation	15-25ppm for 15min or 40-80ppm for 1-2min irritating; 200-400ppm* may cause headache, dizziness, drowsiness, nausea, intoxication
Ingestion	not known; probably irritating to mouth & throat; ingestion likely to cause symptoms similar to inhalation (<i>above</i>) – not a route of industrial exposure * <i>A high concentration is unlikely to occur in an industrial setting.</i>

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 (<i>a type not seen in ♀rats or humans</i>); 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
LD ₅₀ (oral)	1870, 2000, 2145, 2400 & 3450mg/kg (rat), 2000, 2200 & 2690mg/kg (mouse), 1420mg/kg (rabbit), 700mg/kg (guinea pig)
LD ₅₀ (skin)	1390mg/kg (rat), 1380 & 3160mg/kg (rabbit)
LC ₅₀ (inhalation)	1240ppm (rat), 815ppm** (guinea pig), **600ppm is the maximum isophorone vapour concentration of @ 25°C. The above exposures must be to vapour & mist combined, & may not be accurately measurable.

12. ECOLOGICAL INFORMATION

Bioaccumulation	not a bioaccumulator
Biodegradation	biodegrades in the presence of oxygen: 100% in 21days, 95% in 28days, 10% in 22days, 42% in 20days, 100% in 7days & others
Abiotic Degradation	reacts with atmospheric hydroxyl radicals; ½-life in air is 5hrs & 40min (<i>2 tests</i>)
Mobility in soil, water	water soluble, moves readily in soil and water
Aquatic Toxicity	
LC ₅₀ (Fish, 96hr)	140 & 170-300mg/litre (Cyprinodon variegatus), 145, 228 & 255mg/litre (Pimephelas promelas), 220 & 240mg/litre (Lepomis macrochirus)
EC ₅₀ (Crustacea, 48hr)	117 & 120mg/litre (Daphnia magna), 430mg/litre (Artemia salina – 24hr)
EC ₅₀ (Algae)	475mg/litre (Scenedesmus subspicatus), 126mg/litre (Selenastrum capricornutum), 38mg/litre (Champia parvula)
EC ₅₀ (Bacteria)	100mg/litre (domestic sewage sludge), 420mg/litre (Tetrahymena pyriformis)
EC ₁₀ (Bacteria)	328mg/litre (Pseudomonas putida) – <i>NOTE: this is an EC₁₀, not an EC₅₀</i>

13. 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>

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14. TRANSPORT CLASSIFICATION

Canada TDG AND U.S.A. 49 CFR Marine Pollutant ERAP Required	PIN Shipping Name Class & Packing Group	UN – not regulated for transport not regulated for transport not regulated for transport not a marine pollutant NO
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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

Europe Classification

Harmful



Europe Risk Phrases

R: 21/22, 36/37, 40 – Harmful in contact with skin & if swallowed. Irritating to eyes & respiratory system. Limited evidence of a carcinogenic effect

Europe Safety Phrases

S: 13, 23, 36/37/39, 46 – Keep away from food, drink and animal feedstuffs. Do not breathe vapour or spray. Wear suitable protective gloves & eye protection. If swallowed, seek medical advice immediately.

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 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.

16. OTHER INFORMATION

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

Data from RTECS, HSDB (Haz. Substance Data Base), Cheminfo (CCOHS), IUCLID Datasheets (ESIS – European Chem. Substance Info. System), & others.

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