



Isophorone

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Date of issue: 05/30/2015 Version: 1.0

SECTION 1: Identification

1.1. Identification

Product form : Substance
Substance name : Isophorone
CAS-No. : 78-59-1
Product code : (US) W01780
Formula : C9H14O
Synonyms : 1,5,5-Trimethyl-1-cyclohexen-3-one / 3,5,5-Trimethylcyclohex-2-en-1-one / 1,5,5-Trimethylcyclohexen-3-one / 3,5,5-Trimethylcyclohex-2-enone / 1,1,3-Trimethyl-3-cyclohexene-5-one / 3,5,5-Trimethyl-2-cyclohexene-1-one / 3,5,5-Trimethyl-2-cyclohexen-1-one / 1,5,5-Trimethylcyclohexenone / 2-Cyclohexen-1-one, 3,5,5-trimethyl- / Cyclohex-2-en-1-one, 3,5,5-trimethyl- / 3,5,5-Tetramethylcyclohex-2-en-1-one / Isoforone / 3,5,5-Trimethyl-2-cyclohexen-1-on / 1,5,5-Trimethylcyclohexenone-3

1.2. Recommended use and restrictions on use

No additional information available

1.3. Supplier

Synerzine
5340 Hwy 42 S
Ellenwood, Georgia 30294 - USA
T 404-524-6744 - F 404-577-1651
info@synerzine.com - www.synerzine.com

1.4. Emergency telephone number

Emergency number : Infotrac 1-800-535-5053 (Contract# 102471) Dial +1-352-323-3500 when outside the US

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification

Acute toxicity (oral) Category 4	H302	Harmful if swallowed
Acute toxicity (dermal) Category 4	H312	Harmful in contact with skin
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation
Carcinogenicity Category 2	H351	Suspected of causing cancer (Dermal, Inhalation, oral)
Specific target organ toxicity (single exposure) Category 3	H335	May cause respiratory irritation

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

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 (Dermal, Inhalation, oral)

Precautionary statements (GHS-US) :

P201 - Obtain special instructions before use.
P202 - Do not handle until all safety precautions have been read and understood.
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.

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P280 - Wear eye protection, face 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 first aid measures 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.
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
P405 - Store locked up.
P501 - Dispose of contents/container to an approved waste disposal plant

2.3. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	GHS-US classification
Isophorone (Main constituent)	(CAS-No.) 78-59-1	97 - 100	Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Eye Irrit. 2A, H319 Carc. 2, H351 STOT SE 3, H335

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general : IF exposed or concerned: Get medical advice/attention. Call a poison center/doctor/physician if you feel unwell.
First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. Call a poison center/doctor/physician if you feel unwell.
First-aid measures after skin contact : Wash skin with plenty of water. Take off contaminated clothing.
First-aid measures after eye contact : Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion : Rinse mouth. Call a poison center/doctor/physician if you feel unwell.

4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects after inhalation : May cause respiratory irritation.
Symptoms/effects after eye contact : Eye irritation.

4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

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

5.2. Specific hazards arising from the chemical

Reactivity : The product is non-reactive under normal conditions of use, storage and transport.

5.3. Special protective equipment and precautions for fire-fighters

Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

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SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Avoid breathing fume, gas, mist, spray, vapors. Avoid contact with skin, eyes and clothing.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Take up liquid spill into absorbent material. Notify authorities if product enters sewers or public waters.

Other information : Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Wear personal protective equipment. Use only outdoors or in a well-ventilated area. Avoid breathing fume, gas, mist, spray, vapors. Do not get in eyes, on skin, or on clothing.

Hygiene measures : Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store locked up. Store in a well-ventilated place. Keep container tightly closed. Keep cool.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Isophorone (78-59-1)		
ACGIH	Local name	Isophorone
ACGIH	ACGIH Ceiling (ppm)	5 ppm
ACGIH	Remark (ACGIH)	Eye & URT irr; CNS impair;
OSHA	OSHA PEL (TWA) (mg/m ³)	140 mg/m ³
OSHA	OSHA PEL (TWA) (ppm)	25 ppm
IDLH	US IDLH (ppm)	200 ppm
NIOSH	NIOSH REL (TWA) (mg/m ³)	23 mg/m ³
NIOSH	NIOSH REL (TWA) (ppm)	4 ppm

8.2. Appropriate engineering controls

Appropriate engineering controls : Ensure good ventilation of the work station.

Environmental exposure controls : Avoid release to the environment.

8.3. Individual protection measures/Personal protective equipment

Hand protection:

Protective gloves

Eye protection:

Safety glasses

Skin and body protection:

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Wear suitable protective clothing

Respiratory protection:

In case of insufficient ventilation, wear suitable respiratory equipment

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Colorless liquid.
Color	: Colorless
Odor	: sweet, cedarwood, tobacco aroma
Odor threshold	: 0.19 ppm (Hellman and Small) 1.1 mg/m ³ (Hellman and Small)
pH	: No data available
Melting point	: -8.1 °C
Freezing point	: No data available
Boiling point	: 213 - 214 °C
Flash point	: 204 °F TCC
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: Not applicable.
Vapor pressure	: 0.4 hPa (at 20 °C)
Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Specific gravity / density	: 0.922 - 0.932 g/cm ³
Molecular mass	: 138.21 g/mol
Solubility	: Slightly soluble in water. oils. Water: 12 g/l (at 20 °C)
Log Pow	: 1.66 (at 23 °C)
Auto-ignition temperature	: 460 °C
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

None under recommended storage and handling conditions (see section 7).

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

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 mg/kg body weight
ATE US (dermal)	1700 mg/kg body weight
ATE US (vapors)	7 mg/l/4h
ATE US (dust, mist)	7 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 (Dermal, Inhalation, oral).

Isophorone (78-59-1)

National Toxicology Program (NTP) Status	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
Symptoms/effects after inhalation	: May cause respiratory irritation.
Symptoms/effects after eye contact	: Eye irritation.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

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])

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

Isophorone (78-59-1)	
BCF fish 1	7
Log Pow	1.66 (at 23 °C)

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Isophorone (78-59-1)	
1990 Hazardous Air Pollutant (Clean Air Act)	Yes

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SECTION 13: Disposal considerations

13.1. Disposal methods

- Regional legislation (waste) : U.S. - RCRA (Resource Conservation & Recovery Act) - List for Hazardous Constituents. U.S. - RCRA (Resource Conservation & Recovery Act) - TSD Facilities Ground Water Monitoring.
- Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

- Transport document description : NA3082 Hazardous waste, liquid, n.o.s., 9, III
- UN-No.(DOT) : NA3082
- Proper Shipping Name (DOT) : Hazardous waste, liquid, n.o.s.
- Class (DOT) : 9 - Class 9 - Miscellaneous hazardous material 49 CFR 173.140
- Packing group (DOT) : III - Minor Danger
- Hazard labels (DOT) : 9 - Class 9 (Miscellaneous dangerous materials)



- 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).
T2 - 1.5 178.274(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) : 155
- DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : No limit
- DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : No limit
- DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
- Other information : No supplementary information available.

Transportation of Dangerous Goods

Transport by sea

- Transport document description (IMDG) : UN 3082 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., 9, III
- UN-No. (IMDG) : 3082
- Proper Shipping Name (IMDG) : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
- Class (IMDG) : 9 - Miscellaneous dangerous substances and articles
- Packing group (IMDG) : III - substances presenting low danger
- Limited quantities (IMDG) : 5 L

Air transport

- Transport document description (IATA) : UN 3082 Environmentally hazardous substance, liquid, n.o.s., 9, III
- UN-No. (IATA) : 3082

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Proper Shipping Name (IATA)	: Environmentally hazardous substance, liquid, n.o.s.
Class (IATA)	: 9 - Miscellaneous Dangerous Goods
Packing group (IATA)	: III - Minor Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

Isophorone (78-59-1)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

CERCLA RQ	5000 lb
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15.2. International regulations

CANADA

Isophorone (78-59-1)

Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

Isophorone (78-59-1)

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

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 Japanese ISHL (Industrial Safety and Health Law)
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 INSQ (Mexican National Inventory of Chemical Substances)
Listed on CICR (Turkish Inventory and Control of Chemicals)
Listed on the TCSI (Taiwan Chemical Substance Inventory)

15.3. US State regulations

Isophorone (78-59-1)

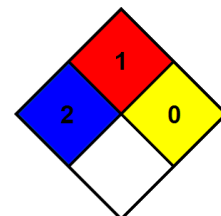
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List U.S. - Pennsylvania - RTK (Right to Know) List
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SECTION 16: Other information

Full text of H-phrases:

H302	Harmful if swallowed
H312	Harmful in contact with skin
H319	Causes serious eye irritation
H335	May cause respiratory irritation
H351	Suspected of causing cancer

NFPA health hazard	: 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.
NFPA fire hazard	: 1 - Materials that must be preheated before ignition can occur.
NFPA reactivity	: 0 - Material that in themselves are normally stable, even under fire conditions.



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Hazard Rating

- Health : 2 Moderate Hazard - Temporary or minor injury may occur
- Flammability : 1 Slight Hazard - Materials that must be preheated before ignition will occur. Includes liquids, solids and semi solids having a flash point above 200 F. (Class IIIB)
- Physical : 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.
- Personal protection : C
C - Safety glasses, Gloves, Synthetic apron

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This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product