SAFETY DATA SHEETS

According to the UN GHS revision 8

Version: 1.0
Creation Date: July 15, 2019
Revision Date: July 15, 2019

1. SECTION 1: Identification

1.1. GHS Product identifier

Product name 3,5,5-trimethylcyclohex-2-enone

1.2. Other means of identification

Product number -

Other names Isooctopherone; Izoforon; 3,5,5-trimethylcyclohex-2-en-1-one

1.3. Recommended use of the chemical and restrictions on use

Identified uses Isophorone is used mainly as a solvent for concentrated vinyl chloride/acetate-based coating systems for metal cans, other metal paints, nitrocellulose finishes, and printing inks for plastics. Isophorone is also used in some herbicide and pesticide formulations and in adhesives for plastics, polyvinylchloride, and polystyrene materials. Isophorone is an intermediate in the synthesis of 3,5-xylenol, 3,3,5-trimethylcyclohexanol, and plant growth retardants.

Uses advised against no data available

1.4. Supplier's details

Company Shandong Sincere Chemical Co., Ltd.

Address No.21 Industrial North Road, Licheng District, Jinan City, Shandong Province, China

Telephone (+86) 188-6575-9396

1.5. Emergency phone number

Emergency phone number (+86) 188-6575-9396

Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

2. SECTION 2: Hazard identification

2.1. Classification of the substance or mixture

Acute toxicity - Category 4, Oral
Acute toxicity - Category 4, Dermal
Eye irritation, Category 2
Specific target organ toxicity – single exposure, Category 3
Carcinogenicity, Category 2

2.2. GHS label elements, including precautionary statements

Pictogram(s)	
Signal word	Warning
Hazard statement(s)	H302 Harmful if swallowedH312 Harmful in contact with skinH319 Causes serious eye irritationH335 May cause respiratory irritationH351 Suspected of causing cancer
Precautionary statement(s)	
Prevention	P264 Wash ... thoroughly after handling.P270 Do not eat, drink or smoke when using this product.P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...P261 Avoid breathing dust/fume/gas/mist/vapours/spray.P271 Use only outdoors or in a well-ventilated area.P203 Obtain, read and follow all safety instructions before use.
Response	P301+P317 IF SWALLOWED: Get medical help.P330 Rinse mouth.P302+P352 IF ON SKIN: Wash with plenty of water/...P317 Get medical help.P321 Specific treatment (see ... on this label).P362+P364 Take off contaminated clothing and wash it before reuse.P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.P319 Get medical help if you feel unwell.P318 IF exposed or concerned, get medical advice.
Storage	P403+P233 Store in a well-ventilated place. Keep container tightly closed.P405 Store locked up.
Disposal	P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3. Other hazards which do not result in classification

no data available

3. SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
3,5,5-trimethylcyclohex-2-enone	3,5,5-trimethylcyclohex-2-enone	78-59-1	201-126-0	99.0%

4. SECTION 4: First-aid measures

4.1. Description of necessary first-aid measures

Medical attention is required. Consult a doctor. Show this safety data sheet (SDS) to the doctor in attendance.

If inhaled

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

Following skin contact

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

Following eye contact

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

Following ingestion

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

4.2. Most important symptoms/effects, acute and delayed

LIQUID: Irritating to skin and eyes. Harmful if swallowed. (USCG, 1999)

4.3. Indication of immediate medical attention and special treatment needed, if necessary

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary . For contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Ketones and related compounds

5. SECTION 5: Fire-fighting measures

5.1. Suitable extinguishing media

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.

5.2. Specific hazards arising from the chemical

Combustible. (USCG, 1999)

5.3. Special protective actions for fire-fighters

Use water spray, powder, foam, carbon dioxide.

6. SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

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.

6.2. Environmental precautions

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.

6.3. Methods and materials for containment and cleaning up

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

7. SECTION 7: Handling and storage

7.1. Precautions for safe handling

NO open flames. Above 84°C use a closed system and ventilation.
Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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.

8. SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Occupational Exposure limit values

TLV: 5 ppm as STEL; A3 (confirmed animal carcinogen with unknown relevance to humans).MAK: 11 mg/m3, 2 ppm; peak limitation category: I(2); carcinogen category: 3B; pregnancy risk group: C

Biological limit values

no data available

8.2. Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3. Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles.
Skin protection
Protective gloves.
Respiratory protection
Use ventilation, local exhaust or breathing protection.
Thermal hazards
no data available

9. SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Liquid.
Colour	None.
Odour	Peppermint-like odor
Melting point/freezing point	-8.1 °C.
Boiling point or initial boiling point and boiling range	215.3 °C. Atm. press.:1 013 hPa.
Flammability	Class IIIA Combustible Liquid: Fl.P. at or above 140°F and below 200°F.
Lower and upper explosion limit/flammability limit	Lower 0.8% by vol; upper 3.8%
Flash point	85 °C. Atm. press.:Ca. 1 013 hPa.
Auto-ignition temperature	470 °C. Atm. press.:Ca. 1 013 hPa.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	kinematic viscosity (in mm^2/s) = 2.83. Temperature:20°C.
Solubility	0.1 to 1 mg/mL at 64° F (NTP, 1992)
Partition coefficient n-octanol/water	log Pow = 1.67. Temperature:20 °C. Remarks:PH not reported (not relevant for non-dissociating substance).
Vapour pressure	0.4 hPa. Temperature:20 °C. Remarks:For values at other temperatures see below.
Density and/or relative density	921.5 kg/m^3. Temperature:20 °C.
Relative vapour density	4.77 (vs air)
Particle characteristics	no data available

10. SECTION 10: Stability and reactivity

10.1. Reactivity
Reacts with strong oxidants, strong bases and amines.

10.2. Chemical stability
no data available

10.3. Possibility of hazardous reactions

Flammable & explosive when exposed to heat or flame.Ketones, such as ISOPHORONE, are reactive with many acids and bases liberating heat and flammable gases (e.g., H2). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H2) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO3, HNO3 + H2O2, and HClO4. Forms explosive peroxides

10.4. Conditions to avoid

no data available

10.5. Incompatible materials

Incompatible with strong oxidizers

10.6. Hazardous decomposition products

no data available

11. SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - 1 500 mg/kg bw.
  Remarks:LD50 confidence limits: 1400-1800 mg/kg.
- Inhalation: LC50 - rat (male) - 7 mg/L air.
- Dermal: LD50 - rabbit (male/female) - 1 200 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Cancer Classification: Group C Possible Human Carcinogen

Reproductive toxicity

No studies were located regarding developmental or reproductive effects in humans. (-) Limited evidence in animal studies suggests that isophorone may cause birth defects such as fetal malformations and growth retardation from inhalation exposure to isophorone during pregnancy.

STOT-single exposure

The substance and the vapour are irritating to the eyes and respiratory tract. The substance may cause effects on the central nervous system.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

12. SECTION 12: Ecological information

12.1. Toxicity

- Toxicity to fish: LC50 - Pimephales promelas - 228 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: NOEC - Daphnia magna - 15 mg/L - 48 h.
- Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 475 mg/L - 72 h.
- Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - 100 mg/L - 3 h. Remarks:Respiration rate.

12.2. Persistence and degradability

AEROBIC: Isophorone, present at 100 mg/l, reached 3% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/l and the Japanese MITI test(1). Removal of isophorone from unacclimated fresh and salt water seeded with settled domestic wastewater was 42 and 9%, respectively, after 20 days(3). Removal of isophorone from wastewater treated by various different biological treatment processes: trickling filter, activated sludge, aerated lagoon, and facultative lagoon was 19, 98, 24, and 30%, respectively(4); therefore this compound is not expected to biodegrade rapidly(SRC). A 100% loss was observed when 5 and 10 mg/l isophorone underwent a 7-day static incubation in the dark at 25 deg C under aerobic conditions using settled domestic wastewater as inoculum(2). Using a multi-level respirometric test protocol employing a sludge microbiota, a half-life of 25 days for 100 mg test compound was determined(5).

12.3. Bioaccumulative potential

A BCF of 7 was measured for isophorone in bluegill sunfish(1). The half-life of isophorone in fish tissue was found to be 1 day(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4. Mobility in soil

The Koc of isophorone is estimated as 200(SRC), using a log Kow of 1.7(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that isophorone is expected to have moderate mobility in soil.

12.5. Other adverse effects

no data available

13. SECTION 13: Disposal considerations

13.1. Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

14. SECTION 14: Transport information

14.1. UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.2. UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.3. Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.4. Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.5. Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

14.6. Special precautions for user

no data available

14.7. Transport in bulk according to IMO instruments

no data available

15. SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
3,5,5-trimethylcyclohex-2-enone	3,5,5-trimethylcyclohex-2-enone	78-59-1	201-126-0
European Inventory of Existing Commercial Chemical Substances (EINECS)	Listed.		
EC Inventory	Listed.		

United States Toxic Substances Control Act (TSCA) Inventory	Listed.
China Catalog of Hazardous chemicals 2015	Not Listed.
New Zealand Inventory of Chemicals (NZIoC)	Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Listed.
Vietnam National Chemical Inventory	Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Listed.
Korea Existing Chemicals List (KECL)	Listed.

16. SECTION 16: Other information

Information on revision

Creation Date July 15, 2019
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Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Other Information

The occupational exposure limit value should not be exceeded during any part of the working exposure.

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. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product.