

According to the UN GHS revision 9

Version: 1.0
Creation Date: July 15, 2019
Revision Date: July 15, 2019**SECTION 1: Identification****1.1 GHS Product identifier**

Product name 4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one

1.2 Other means of identification

Product number -

Other names 4-(2,6,6-Trimethyl-2-cyclohexenyl)-3-buten-2-one;alpha-ionone;4-(2,6,6-Trimethylcyclohex-2-en-1-yl)but-3-en-2-one

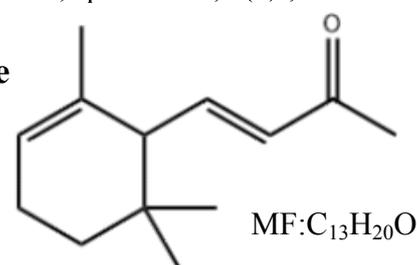
1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research use.

Uses advised against no data available

1.4 Supplier's details

Company Jiangxi LinQ Spices Co.,Ltd.
Address Building15#,Xinghai Gardon,TianLi Square,QingYuan District,
Ji'An City,JiangXi Province
Telephone (+86)0796-8287629

**SECTION 2: Hazard identification****2.1 Classification of the substance or mixture**

Not classified.

2.2 GHS label elements, including precautionary statements

Pictogram(s) No symbol.
Signal word No signal word
Hazard statement(s) none
Precautionary statement(s)
Prevention none
Response none
Storage none
Disposal none

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients**3.1 Substances**

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one	4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one	127-41-3	204-841-6	100%

SECTION 4: First-aid measures**4.1 Description of necessary first-aid measures**

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

4.2 Most important symptoms/effects, acute and delayed

no data available

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Poisons A and B

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Specific hazards arising from the chemical

no data available

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

6.2 Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.; Environmental precautions: Do not let product enter drains.; Methods and materials for containment and cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

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

Conditions for safe storage, including any incompatibilities: Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Light sensitive.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Liquid. Liquid.
Colour	Pale yellow.
Odour	It has a warm, woody, floral odor with balsamic and sweet tones and is strongly reminiscent of violet flowers.
Melting point/freezing point	-13.7 °C. Atm. press.:965.7 hPa. Remarks:Freezing point less than -13.7 °C ,No freezing was observed up to -13.7 °C.
Boiling point or initial boiling point and boiling range	207.7 °C. Atm. press.:968.6 hPa.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	87.3 °C. Atm. press.:973 hPa.
Auto-ignition temperature	Atm. press.:995 hPa. Remarks:4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one did not catch fire on being exposed to air at room temperature of 23 degC.
Decomposition temperature	no data available
pH	4.55. Remarks:No other detail available.
Kinematic viscosity	kinematic viscosity (in mm ² /s) = 41.15. Temperature:20°C. Remarks:No other detail available.;kinematic viscosity (in mm ² /s) = 28.405. Temperature:40°C. Remarks:No other detail available.;dynamic viscosity (in mPa s) = 36.45. Temperature:20°C. Remarks:No other detail available.
Solubility	In water, 106 mg/L at 25 deg C
Partition coefficient n-octanol/water	log Pow = 3.85. Remarks:Log Pow = 3.85 with a standard error of 0.08.
Vapour pressure	3.61 Pa. Temperature:25 °C. Remarks:3.61 Pa = 0.0271 mm Hg at 25 deg C, estimated data.
Density and/or relative density	0.916 g/cm ³ . Temperature:23 °C.
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Incompatible materials: Strong oxidizing agents.

10.6 Hazardous decomposition products

Special hazards arising from the substance or mixture: Carbon oxides

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

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

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 10.939 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 10 mg/L - 48 h.
- Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 9.27 mg/L - 72 h.
- Toxicity to microorganisms: NOEC - *Pseudomonas aeruginosa* - 1 278 mg/dish - 10 d.

12.2 Persistence and degradability

AEROBIC: The biodegradability of alpha-ionone is expected to be analogous to beta-ionone(SRC). Using the OECD 301F method (manometric respirometry) with an activated sludge inoculum, beta-ionone, at 50 mg/L, reached 79% of its theoretical BOD in 28 days which classified the compound as readily biodegradable(1). beta-ionone was also classified as readily biodegradable by the results of a CO₂-evolution test where beta-ionone, at 10 mg/L, achieved 46% and 73% CO₂ evolution after 7 and 28 days respectively(1). Another respirometry study reported 80% biodegradation of beta-ionone at 100 mg/L(2). In a spiked river water die-away test using water from the Murrumbidgee River, beta-ionone, at 6.28 ug/L, was degraded about 95% after 20 hours of incubation(1). Results of a modified MITI test (OECD 301C) reported 50% degradation of beta-ionone after 28 days (consistent with inherent biodegradability), but concentrations or inoculum were not reported(1).

12.3 Bioaccumulative potential

An estimated BCF of 161 was calculated in fish for alpha-ionone(SRC), using a log K_{ow} of 3.85(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC), provided the compound is not metabolized by the organism(SRC).

12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the K_{oc} of alpha-ionone can be estimated to be 670(SRC). According to a classification scheme(2), this estimated K_{oc} value suggests that alpha-ionone is expected to have low mobility in soil.

12.5 Other adverse effects

no data available

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.

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.) (For 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.) (For 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.) (For 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.) (For 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

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
4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one	4-(2,6,6-trimethylcyclohex-2-ene-1-yl)-but-3-ene-2-one	127-41-3	204-841-6
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.

SECTION 16: Other information

Information on revision

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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/>

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