

According to the UN GHS revision 8

Creation Date: April 30, 2026

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1. IDENTIFICATION

1.1 GHS Product identifier

Product name: (E)- β -Ionone

Catalog Number: TN2999

CAS Number: 79-77-6

1.2 Other means of identification

Other names: -

1.3 Recommended use of the chemical and restrictions on use

Identified uses:

1.4 Supplier's details

Company: Targetmol Chemicals Inc.

Address: 34 Washington Street, Wellesley Hills, Massachusetts 02481 USA

Tel/Fax: (781) 999-4286

1.5 Emergency phone number

Emergency phone number: 781-999-4286

Service hours: Monday to Friday, 9am-5pm (Standard timezone: UTC/GMT -5 hours).

2. HAZARD IDENTIFICATION

2.1 Classification of the substance or mixture

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

2.2 GHS label elements, including precautionary statements

Pictogram(s):



Signal word: No signal word

Hazard statement(s): H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s):

Prevention: P273 Avoid release to the environment.

Response: P391 Collect spillage.

Storage: none

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. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number
(E)- β -Ionone	-	79-77-6	201-224-3

4. FIRST-AID MEASURES

4.1 Description of necessary first-aid measures

General advice

no data available

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

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

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

ACUTE/CHRONIC HAZARDS: Toxic. May cause allergic reaction. (NTP, 1992)

5. FIRE-FIGHTING MEASURES

5.1 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.

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.; Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.; 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.

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.

Pure form: -20°C for 3 years | In solvent: -80°C for 1 year

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/flame 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

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state	Solid
Color	no data available
Odour	Warm woody, dry, and fruity odor
Melting point/freezing point	-35 °C. Atm. press.:1 013 hPa.
Boiling point or initial boiling point and boiling range	267.1 °C. Atm. press.:1 013 hPa. Remarks:Extrapolated.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	126 °C. Atm. press.:1 013.25 hPa.
Auto-ignition temperature	273 °C. Atm. press.:1 010 - 1 017 hPa.
Decomposition temperature	no data available

pH	no data available
Kinematic viscosity	dynamic viscosity (in mPa s) = 11.2. Temperature:20°C.;dynamic viscosity (in mPa s) = 5.04. Temperature:40°C.;kinematic viscosity (in mm ² /s) = 11.8. Temperature:20°C.
Solubility	DMSO: 100 mg/mL (520.02 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
N-octanol-water partition coefficient	log Pow = 4. Temperature:25 °C.
Vapour pressure	Ca. 0.072 hPa. Temperature:25 °C.
Density and/or relative density	0.945 g/cm ³ at 25°C (lit.)
Relative vapour density	no data available
Particle characteristics	no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

Slightly water soluble (NTP, 1992).

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Combustible liquid.BETA-IONONE may react vigorously with oxidizing agents. May react exothermically with reducing agents to release hydrogen gas.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Incompatible materials: Strong oxidizing agents.

10.6 Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral: LD50 - rat - 7 120 mg/kg bw. Remarks:+/- 1000 mg/kg bw for deaths occurring within 24 h.

Inhalation: no data available

Dermal: LD50 - rat (male/female) - > 2 000 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

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 5.09 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 4.03 mg/L - 48 h.

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 22.15 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - 100 - 200 mg/L - 180 min. Remarks: Respiration rate.

12.2 Persistence and degradability

AEROBIC: 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 after 28 days (consistent with inherent biodegradability), but concentrations or inoculum were not reported(1).

12.3 Bioaccumulative potential

An estimated BCF of 202 was calculated in fish for beta-ionone(SRC), using a log Kow of 4.0(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 Koc of beta-ionone can be estimated to be 670(SRC). According to a classification scheme(2), this estimated Koc value suggests that beta-ionone is expected to have low mobility in soil.

12.5 Other adverse effects

no data available

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. TRANSPORT INFORMATION

14.1 UN Number

no data available

14.2 UN Proper Shipping Name

no data available

14.3 Transport hazard class(es)

no data available

14.4 Packing group, if applicable

no data available

14.5 Environmental hazards

no data available

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

15. REGULATORY INFORMATION

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

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. 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>

A DRUG SCREENING EXPERT

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

no data available

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