

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : β -Ionone

Product Number : I12603
Brand : Aldrich

Supplier : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

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Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards

No known OSHA hazards

GHS Classification

Acute aquatic toxicity (Category 2)

GHS Label elements, including precautionary statements

Pictogram : none

Signal word : none

Hazard statement(s)
H401 : Toxic to aquatic life.

Precautionary statement(s) : none

HMIS Classification

Health hazard: 0
Flammability: 1
Physical hazards: 0

NFPA Rating

Health hazard: 0
Fire: 1
Reactivity Hazard: 0

Potential Health Effects

Inhalation : May be harmful if inhaled. May cause respiratory tract irritation.
Skin : May be harmful if absorbed through skin. May cause skin irritation.
Eyes : May cause eye irritation.
Ingestion : May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-buten-2-one
beta-Ionone

Formula : C₁₃H₂₀O

Molecular Weight : 192.30 g/mol

No ingredients are hazardous according to OSHA criteria.

4. FIRST AID MEASURES

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Conditions of flammability

Not flammable or combustible.

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

Avoid breathing vapours, 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

Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Conditions for safe storage

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.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection

Respiratory protection not required. For nuisance exposures use type OV/AG (US) or type ABEK (EU EN 14387) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Eye protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection

impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9. PHYSICAL AND CHEMICAL PROPERTIES**Appearance**

Form	clear, liquid
Colour	light yellow

Safety data

pH	7
Melting point/freezing point	-35 °C (-31 °F) at 1,013 hPa (760 mmHg)
Boiling point	126 - 128 °C (259 - 262 °F) at 16 hPa (12 mmHg) - lit.
Flash point	112 °C (234 °F) - closed cup
Ignition temperature	no data available
Auto-ignition temperature	273 °C (523 °F) at 1,010 - 1,017 hPa (758 - 763 mmHg)
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	ca.0.072 hPa (0.054 mmHg) at 25 °C (77 °F)
Density	0.945 g/cm ³ at 25 °C (77 °F)
Water solubility	0.11 g/l at 20 °C (68 °F) - OECD Test Guideline 105
Partition coefficient: n-octanol/water	log Pow: 4 at 25 °C (77 °F)
Viscosity, kinematic	11.2 mm ² /s at 20 °C (68 °F)
Relative vapour density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY**Chemical stability**

Stable under recommended storage conditions.

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Materials to avoid

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION**Acute toxicity****Oral LD50**

LD50 Oral - rat - 7,120 mg/kg

Inhalation LC50

no data available

Dermal LD50

LD50 Dermal - rat - male and female - > 2,000 mg/kg

Other information on acute toxicity

no data available

Skin corrosion/irritation

Skin - rabbit - No skin irritation - 4 h - OECD Test Guideline 404

Serious eye damage/eye irritation

Eyes - rabbit - No eye irritation - 72 h - OECD Test Guideline 405

Respiratory or skin sensitisation

guinea pig - Does not cause skin sensitisation. - OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vitro - Ames test - S. typhimurium - with and without metabolic activation - negative

Genotoxicity in vivo - mouse - male - Intraperitoneal - negative

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

Reproductive toxicity - Hamster - Oral

Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Teratogenicity**Specific target organ toxicity - single exposure (Globally Harmonized System)**

no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)

no data available

Aspiration hazard

no data available

Potential health effects**Inhalation**

May be harmful if inhaled. May cause respiratory tract irritation.

Ingestion May be harmful if swallowed.
Skin May be harmful if absorbed through skin. May cause skin irritation.
Eyes May cause eye irritation.

Signs and Symptoms of Exposure

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Synergistic effects

no data available

Additional Information

Repeated dose toxicity - rat - female - Oral - No observed adverse effect level - 83 mg/kg - Lowest observed adverse effect level - 801 mg/kg
RTECS: EN0500000

12. ECOLOGICAL INFORMATION

Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 5.09 mg/l - 96.0 h
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 4.03 mg/l - 48 h Method: OECD Test Guideline 202
Toxicity to algae	static test EC50 - Desmodesmus subspicatus (green algae) - 22.15 mg/l - 72 h
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - 100 - 200 mg/l - 180 min Method: OECD Test Guideline 209

Persistence and degradability

Biodegradability aerobic
Result: 70 - 80 % - Readily biodegradable.

Bioaccumulative potential

no data available

Mobility in soil

no data available

PBT and vPvB assessment

no data available

Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards

No known OSHA hazards

SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

No SARA Hazards

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
(E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-77-6	

New Jersey Right To Know Components

	CAS-No.	Revision Date
(E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	79-77-6	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Further information

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