

SAFETY DATA SHEET

1. PRODUCT

1.1 Product identifiers

Name: -Ionone

CAS-No.: 79-77-6

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute aquatic toxicity (Category 2), H401

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram	N/A
Signal word	none
Hazard statement(s)	H401 Toxic to aquatic life.
Precautionary statement(s)	P273 Avoid release to the environment. P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

No data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula: $C_{13}H_{20}O$

Molecular weight: 192.3 g/mol

CAS-No.: 79-77-6

EC-No.: 201-224-3

No components need to be disclosed according to the applicable regulations.

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of 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.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.2 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Avoid breathing vapours, mist or gas. Ensure adequate ventilation.

For personal protection see section 8.

6.2 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.

6.3 Methods and materials for containment and cleaning up

Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 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.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Skin 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.
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.
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).
Control of environmental exposure	Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Appearance	Form: clear, liquid Colour: light yellow
Odour	No data available
Odour Threshold	No data available
pH	7
Melting point/freezing point	-35 °C (-31 °F) at 1,013 hPa (760 mmHg)
Initial boiling point and boiling range	126 - 128 °C (259 - 262 °F) at 16 hPa (12 mmHg) 266 - 269 °C (511 - 516 °F) at 1,013 hPa (760 mmHg)
Flash point	112 °C (234 °F) - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	ca.0.072 hPa (0.054 mmHg) at 25 °C (77 °F)
Vapour density	No data available
Relative density	0.945 g/cm ³
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)
Auto-ignition temperature	273 °C (523 °F) at 1,010 - 1,017 hPa (758 - 763 mmHg)
Decomposition temperature	No data available
Viscosity	11.2 mm ² /s at 20 °C (68 °F) -
Explosive properties	No data available
Oxidizing properties	No data available

9.2 Other safety information

Surface tension: 39.52 mN/m at 20 °C (68 °F)

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

Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 7,120 mg/kg
Inhalation: No data available
LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)
No data available

Skin corrosion/irritation

Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation - 72 h
(OECD Test Guideline 405)

Respiratory or skin sensitisation

- Guinea pig
Result: Does not cause skin sensitisation.
(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test
S. typhimurium
Result: negative
Directive 67/548/EEC, Annex V, B.12.
Mouse - male
Result: 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).

Specific target organ toxicity -single exposure

No data available

Specific target organ toxicity -repeated exposure

No data available

Aspiration hazard

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

12. ECOLOGICAL INFORMATION

12.1 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 (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 (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 70 - 80 % - Readily biodegradable
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

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

Toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

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

SARA 302 Components

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

SARA 313 Components

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

Component	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

Component	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

Full text of H-Statements referred to under sections 2 and 3.

H401 Toxic to aquatic life.

HMIS Rating

Health hazard: 0

Chronic Health Hazard:

Flammability: 1

Physical Hazard 0

NFPA Rating

Health hazard: 0

Fire Hazard: 1

Reactivity Hazard: 0
