

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.0 Revision Date 30.03.2016

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : β -Ionone

Product Number : I12603

Brand : Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Chemie GmbH
Eschenstrasse 5
D-82024 TAUFKIRCHEN

Telephone : +49 (0)89 6513-1130

Fax : +49 (0)89 6513-1161

1.4 Emergency telephone number

Emergency Phone # : 0800 181 7059 (CHEMTREC Deutschland)
+49 (0)696 43508409 (CHEMTREC weltweit)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

2.2 Label elements

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

3.1 Substances

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

Formula : C₁₃H₂₀O

Molecular weight : 192.30 g/mol

CAS-No. : 79-77-6

EC-No. : 201-224-3

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

SECTION 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 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

SECTION 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.

SECTION 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

Store in cool place. 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.

Storage class (TRGS 510): Combustible liquids not in Storage Class 3

7.3 Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

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.

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: clear, liquid
Colour: light yellow |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | 7 |
| e) Melting point/freezing point | -35 °C at 1,013 hPa |
| f) Initial boiling point and boiling range | 126 - 128 °C at 16 hPa - lit. |
| g) Flash point | 112 °C - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapour pressure | ca.0.072 hPa at 25 °C |

l) Vapour density	No data available
m) Relative density	0.945 g/cm ³ at 25 °C
n) Water solubility	0.11 g/l at 20 °C - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	log Pow: 4 at 25 °C
p) Auto-ignition temperature	273 °C at 1,010 - 1,017 hPa
q) Decomposition temperature	No data available
r) Viscosity	11.2 mm ² /s at 20 °C -
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

Surface tension	39.52 mN/m at 20 °C
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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

Strong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 7,120 mg/kg((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

LD50 Dermal - Rat - male and female - > 2,000 mg/kg((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Result: No eye irritation - 72 h

(OECD Test Guideline 405)

Respiratory or skin sensitisation

- Guinea pig((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Result: Does not cause skin sensitisation.

(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

S. typhimurium

Result: negative

Directive 67/548/EEC, Annex V, B.12.((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

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.

Reproductive toxicity

Specific target organ toxicity - single exposure

No data available((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

Additional Information

Repeated dose toxicity - Rat - female - Oral - No observed adverse effect level - 83 mg/kg - Lowest observed adverse effect level - 801 mg/kg((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)
RTECS: EN0500000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 5.09 mg/l - 96.0 h((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 4.03 mg/l - 48 h((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one) (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - Desmodesmus subspicatus (green algae) - 22.15 mg/l - 72 h((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - 100 - 200 mg/l - 180 min((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one) (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)
Result: 70 - 80 % - Readily biodegradable

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available((E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one)

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

Toxic to aquatic life.

SECTION 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.

SECTION 14: Transport information**14.1 UN number**

ADR/RID: -

IMDG: -

IATA: -

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA: -

14.4 Packaging group

ADR/RID: -

IMDG: -

IATA: -

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

No data available

SECTION 15: Regulatory information**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information**Further information**

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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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.