

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.7

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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 :  $\beta$ -Ionone

Product Number : 91036

Brand : Sigma-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

CHEMIKART

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification according to Regulation (EC) No 1272/2008

Long-term (chronic) aquatic hazard (Category 2), H411

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

### 2.2 Label elements

#### Labelling according Regulation (EC) No 1272/2008

Pictogram

|                                                    |                                                                                                                               |
|----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| Signal Word                                        | none                                                                                                                          |
| Hazard statement(s)<br>H411                        | Toxic to aquatic life with long lasting effects.                                                                              |
| Precautionary statement(s)<br>P273<br>P391<br>P501 | Avoid release to the environment.<br>Collect spillage.<br>Dispose of contents/ container to an approved waste disposal plant. |
| Supplemental Hazard Statements                     | none                                                                                                                          |

### Reduced Labeling (<= 125 ml)

Pictogram

|                                |      |
|--------------------------------|------|
| Signal Word                    | none |
| Hazard statement(s)            | none |
| Precautionary statement(s)     | none |
| Supplemental Hazard Statements | none |

### 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                     |
|------------------|-------------------------------------|
| Formula          | : C <sub>13</sub> H <sub>20</sub> O |
| Molecular weight | : 192,3 g/mol                       |
| CAS-No.          | : 79-77-6                           |
| EC-No.           | : 201-224-3                         |

| Component                           | Classification          | Concentration |
|-------------------------------------|-------------------------|---------------|
| <b>trans-β-Ionone</b>               |                         |               |
| CAS-No. 79-77-6<br>EC-No. 201-224-3 | Aquatic Chronic 2; H411 | <= 100 %      |

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### **If inhaled**

After inhalation: fresh air.

#### **In case of skin contact**

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

#### **In case of eye contact**

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### **If swallowed**

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### **Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

### 5.4 Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

## **6.2 Environmental precautions**

Do not let product enter drains.

## **6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.

## **6.4 Reference to other sections**

For disposal see section 13.

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## **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**

#### **Storage conditions**

Tightly closed.

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

### **7.3 Specific end use(s)**

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

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

### **8.2 Exposure controls**

#### **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). Safety glasses

##### **Skin protection**

not required

##### **Respiratory protection**

Not required; except in case of aerosol formation.

##### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Physical state                      oily

|                                                 |                                                                                                                                                                                          |
|-------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| b) Color                                        | yellow                                                                                                                                                                                   |
| c) Odor                                         | No data available                                                                                                                                                                        |
| d) Melting point/freezing point                 | Melting point: -35 °C at 1.013 hPa                                                                                                                                                       |
| e) Initial boiling point and boiling range      | No data available                                                                                                                                                                        |
| f) Flammability (solid, gas)                    | No data available                                                                                                                                                                        |
| g) Upper/lower flammability or explosive limits | No data available                                                                                                                                                                        |
| h) Flash point                                  | 126 °C - closed cup - Tested according to Annex V of Directive 67/548/EEC.                                                                                                               |
| i) Autoignition temperature                     | 273 °C at 1.013 hPa - DIN 51794                                                                                                                                                          |
| j) Decomposition temperature                    | > 215 °C<br>Decomposes on heating.                                                                                                                                                       |
| k) pH                                           | No data available                                                                                                                                                                        |
| l) Viscosity                                    | Viscosity, kinematic: 11,8 mm <sup>2</sup> /s at 20 °C - OECD Test Guideline 1145, 43 mm <sup>2</sup> /s at 40 °C - OECD Test Guideline 114<br><br>Viscosity, dynamic: No data available |
| m) Water solubility                             | 0,11 g/l at 20 °C - OECD Test Guideline 105                                                                                                                                              |
| n) Partition coefficient: n-octanol/water       | log Pow: 4 at 25 °C - Bioaccumulation is not expected.                                                                                                                                   |
| o) Vapor pressure                               | < 1 hPa at 25 °C                                                                                                                                                                         |
| p) Density                                      | 0,95 g/cm <sup>3</sup> at 20 °C                                                                                                                                                          |
| Relative density                                | No data available                                                                                                                                                                        |
| q) Relative vapor density                       | No data available                                                                                                                                                                        |
| r) Particle characteristics                     | No data available                                                                                                                                                                        |
| s) Explosive properties                         | No data available                                                                                                                                                                        |
| t) Oxidizing properties                         | none                                                                                                                                                                                     |

## 9.2 Other safety information

No data available

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## **SECTION 10: Stability and reactivity**

### **10.1 Reactivity**

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### **10.2 Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature) .

### **10.3 Possibility of hazardous reactions**

Violent reactions possible with:  
Strong oxidizing agents

### **10.4 Conditions to avoid**

Strong heating.

### **10.5 Incompatible materials**

No data available

### **10.6 Hazardous decomposition products**

In the event of fire: see section 5

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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

Oral: No data available  
Inhalation: No data available  
Dermal: 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 sensitization**

No data available

#### **Germ cell mutagenicity**

Test Type: Micronucleus test  
Species: Mouse  
Cell type: Bone marrow  
Application Route: Intraperitoneal injection  
Method: OECD Test Guideline 474  
Result: negative

#### **Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information****Endocrine disrupting properties****Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

RTECS: EN0500000

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

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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**SECTION 12: Ecological information****12.1 Toxicity**

|                                                     |                                                                                                                                                                                     |
|-----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Toxicity to fish                                    | static test LC50 - Leuciscus idus (Golden orfe) - 6,81 mg/l - 96 h (DIN 38412)                                                                                                      |
| 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 ErC50 - Desmodesmus subspicatus (green algae) - 22,15 mg/l - 72 h (DIN 38412)<br>static test EC10 - Desmodesmus subspicatus (green algae) - 7,1 mg/l - 72 h (DIN 38412) |
| Toxicity to bacteria                                | static test EC50 - activated sludge - 100 - 200 mg/l - 3 h (OECD Test Guideline 209)                                                                                                |

**12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 28 d

Result: 70 - 80 % - Readily biodegradable.  
(OECD Test Guideline 301F)

### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### 12.6 Endocrine disrupting properties

#### Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

### 12.7 Other adverse effects

No ecological problems are to be expected when the product is handled and used with due care and attention.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 3082

IMDG: 3082

IATA: 3082

### 14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (trans- $\beta$ -Ionone)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (trans- $\beta$ -Ionone)

IATA: Environmentally hazardous substance, liquid, n.o.s. (trans- $\beta$ -Ionone)

### 14.3 Transport hazard class(es)

ADR/RID: 9

IMDG: 9

IATA: 9

### 14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

### 14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: yes

### 14.6 Special precautions for user

Tunnel restriction code : (-)



**Further information**

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

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

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

**National legislation**

Seveso III: Directive 2012/18/EU of the E2 ENVIRONMENTAL HAZARDS  
European Parliament and of the Council  
on the control of major-accident hazards  
involving dangerous substances.

**Other regulations**

Take note of Dir 94/33/EC on the protection of young people at work.

**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

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**SECTION 16: Other information****Full text of H-Statements referred to under sections 2 and 3.**

H411 Toxic to aquatic life with long lasting effects.

## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

## Further information

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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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