

## SAFETY DATA SHEET

Version 6.4  
Revision Date 09/17/2021  
Print Date 02/18/2023**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name :  $\beta$ -IononeProduct Number : I12603  
Brand : Aldrich  
CAS-No. : 14901-07-6**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATESTelephone : +1 314 771-5765  
Fax : +1 800 325-5052**1.4 Emergency telephone**Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**Skin irritation (Category 2), H315  
Short-term (acute) aquatic hazard (Category 2), H401  
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 GHS Label elements, including precautionary statements**

Pictogram



Signal word : Warning

Hazard statement(s)  
H315 : Causes skin irritation.

|                            |   |
|----------------------------|---|
| H411                       | Toxic to aquatic life with long lasting effects.                    |
| Precautionary statement(s) |   |
| P264                       | Wash skin thoroughly after handling.                                |
| P273                       | Avoid release to the environment.                                   |
| P280                       | Wear protective gloves.   |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.                     |
| P332 + P313                | If skin irritation occurs: Get medical advice/ attention.           |
| P362                       | Take off contaminated clothing and wash before reuse.               |
| P391                       | Collect spillage.   |
| P501                       | Dispose of contents/ container to an approved waste disposal plant. |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

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

Formula : C<sub>13</sub>H<sub>20</sub>O  
Molecular weight : 192.30 g/mol  
CAS-No. : 14901-07-6  
EC-No. : 201-224-3

| Component   | Classification  | Concentration |
|---|---|---------------|
| <b>4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one</b> |   |               |
|   | Skin Irrit. 2; Aquatic Acute 2; Aquatic Chronic 2; H315, H401, 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

#### General advice

Consult a physician. Show this material 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

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### **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

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### **SECTION 6: Accidental release measures**

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

Use personal protective equipment. Avoid breathing vapors, 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**

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

#### **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**

##### **Advice on safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

##### **Hygiene measures**

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

For precautions see section 2.2.

#### **7.2 Conditions for safe storage, including any incompatibilities**

##### **Storage conditions**

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**

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**

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**

Safety glasses with side-shields conforming to EN166 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**

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. 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.

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

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

- |               |                   |
|---------------|-------------------|
| a) Appearance | Form: liquid      |
| b) Odor       | No data available |

|   |   |
|---|---|
| c) Odor Threshold                               | No data available   |
| d) pH   | 5.67 at 24 °C (75 °F) - (as aqueous solution)                             |
| e) Melting point/freezing point                 | No data available   |
| f) Initial boiling point and boiling range      | 126 - 128 °C 259 - 262 °F at 16 hPa - lit.                                |
| g) Flash point                                  | > 113 °C (> 235 °F) - 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) Vapor pressure                               | No data available   |
| l) Vapor density                                | No data available   |
| m) Density                                      | 0.945 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.                           |
| Relative density                                | No data available   |
| n) Water solubility                             | 10,000 g/l at 27 °C (81 °F)   |
| o) Partition coefficient: n-octanol/water       | log Pow: 1.90 at 27 °C (81 °F) - (Lit.), Bioaccumulation is not expected. |
| p) Autoignition temperature                     | No data available   |
| q) Decomposition temperature                    | No data available   |
| r) Viscosity                                    | 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

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

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 4,590 mg/kg

Remarks: (RTECS)

Inhalation: No data available

Dermal: No data available

LD50 Intraperitoneal - Mouse - 2,277 mg/kg

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals. The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

#### Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (Lit.)

#### Carcinogenicity

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

NTP: No ingredient 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 on OSHA's list of regulated carcinogens.

#### Reproductive toxicity

No data available

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

RTECS: EN0500000

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

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish                      LC50 - Pimephales promelas (fathead minnow) - 4.7 - 5.4 mg/l - 96 h  
Remarks: (Lit.)

### 12.2 Persistence and degradability

No data available

### 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 with long lasting effects.

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## 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.

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## SECTION 14: Transport information

### DOT (US)

Not dangerous goods

### IMDG

UN number: 3082    Class: 9                      Packing group: III                      EMS-No: F-A, S-F  
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one)  
Marine pollutant : yes

### IATA

UN number: 3082    Class: 9                      Packing group: III  
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one)

### Further information

Aldrich - I12603

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## SECTION 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

|  |                       |               |
|--|-----------------------|---------------|
| 4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one | CAS-No.<br>14901-07-6 | Revision Date |
|--|-----------------------|---------------|

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## SECTION 16: Other information

### Further information

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