

## SAFETY DATA SHEET

Version 6.4  
Revision Date 03/03/2022  
Print Date 05/28/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2,6-Dimethyl-4-heptanone

Product Number : 273848

Brand : Aldrich

Index-No. : 606-005-00-X

CAS-No. : 108-83-8

**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 STATES

Telephone : +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)**

Flammable liquids (Category 3), H226

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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)

H226

Flammable liquid and vapor.

|                            |                                                                                                                             |
|----------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| H335                       | May cause respiratory irritation.                                                                                           |
| Precautionary statement(s) |                                                                                                                             |
| P210                       | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.                                                         |
| P233                       | Keep container tightly closed.                                                                                              |
| P240                       | Ground/bond container and receiving equipment.                                                                              |
| P241                       | Use explosion-proof electrical/ ventilating/ lighting/ equipment.                                                           |
| P242                       | Use only non-sparking tools.                                                                                                |
| P243                       | Take precautionary measures against static discharge.                                                                       |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.                                                                       |
| P271                       | Use only outdoors or in a well-ventilated area.                                                                             |
| P280                       | Wear protective gloves/ eye protection/ face protection.                                                                    |
| P303 + P361 + P353         | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.                        |
| P304 + P340 + P312         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell. |
| P370 + P378                | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.                                        |
| P403 + P233                | Store in a well-ventilated place. Keep container tightly closed.                                                            |
| P403 + P235                | Store in a well-ventilated place. Keep cool.                                                                                |
| P405                       | Store locked up.                                                                                                            |
| P501                       | Dispose of contents/ container to an approved waste disposal plant.                                                         |

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

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                    |
|------------------|------------------------------------|
| Synonyms         | : Diisobutyl ketone<br>Isovalerone |
| Formula          | : C <sub>9</sub> H <sub>18</sub> O |
| Molecular weight | : 142.24 g/mol                     |
| CAS-No.          | : 108-83-8                         |
| EC-No.           | : 203-620-1                        |
| Index-No.        | : 606-005-00-X                     |

| Component                       | Classification                                                                                  | Concentration |
|---------------------------------|-------------------------------------------------------------------------------------------------|---------------|
| <b>2,6-Dimethylheptan-4-one</b> |                                                                                                 |               |
|                                 | Flam. Liq. 3; STOT SE 3;<br>H226, H335<br>Concentration limits:<br>>= 10 %: STOT SE 3,<br>H335; | <= 100 %      |

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

---

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### 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: immediately make victim drink water (two glasses at most). 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

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 at elevated temperatures.

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

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

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

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

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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. Risk of explosion.

### **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.

---

## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on protection against fire and explosion**

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### **Hygiene measures**

Change contaminated clothing. Wash hands after working with substance. 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. Keep away from heat and sources of ignition.

#### **Storage class**

Storage class (TRGS 510): 3: Flammable liquids

### **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**

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

| Component                | CAS-No.  | Value | Control parameters  | Basis                                                                                   |
|--------------------------|----------|-------|---------------------|-----------------------------------------------------------------------------------------|
| 2,6-Dimethylheptan-4-one | 108-83-8 | TWA   | 25 ppm              | USA. ACGIH Threshold Limit Values (TLV)                                                 |
|                          |          | TWA   | 25 ppm<br>150 mg/m3 | USA. NIOSH Recommended Exposure Limits                                                  |
|                          |          | TWA   | 50 ppm<br>290 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants        |
|                          |          | TWA   | 25 ppm<br>150 mg/m3 | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000                           |
|                          |          | PEL   | 25 ppm<br>150 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

## 8.2 Exposure controls

### Appropriate engineering controls

Change contaminated clothing. Wash hands after working with substance.

### 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

required

#### Body Protection

Flame retardant antistatic protective clothing.

#### Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

#### Control of environmental exposure

Do not let product enter drains. Risk of explosion.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                   |                                                                  |
|-------------------|------------------------------------------------------------------|
| a) Appearance     | Form: clear, liquid<br>Color: colorless                          |
| b) Odor           | No data available                                                |
| c) Odor Threshold | No data available                                                |
| d) pH             | No data available                                                |
| e) Melting        | Melting point/freezing point: -45.98 °C (-50.76 °F) at ca.1013.0 |

Aldrich - 273848

Page 5 of 10

|    |                                              |                                                                    |
|----|----------------------------------------------|--------------------------------------------------------------------|
|    | point/freezing point                         | hPa                                                                |
| f) | Initial boiling point and boiling range      | 165 - 170 °C 329 - 338 °F - lit.                                   |
| g) | Flash point                                  | 49 °C (120 °F)                                                     |
| h) | Evaporation rate                             | No data available                                                  |
| i) | Flammability (solid, gas)                    | No data available                                                  |
| j) | Upper/lower flammability or explosive limits | Upper explosion limit: 6.2 %(V)<br>Lower explosion limit: 0.8 %(V) |
| k) | Vapor pressure                               | 2.3 hPa at 20 °C (68 °F)                                           |
| l) | Vapor density                                | 4.91 - (Air = 1.0)                                                 |
| m) | Density                                      | 0.808 g/mL at 25 °C (77 °F) - lit.                                 |
|    | Relative density                             | No data available                                                  |
| n) | Water solubility                             | 0.43 g/l at 25 °C (77 °F) - partly soluble                         |
| o) | Partition coefficient: n-octanol/water       | log Pow: 3.71 at 25 °C (77 °F)                                     |
| p) | Autoignition temperature                     | 345 °C (653 °F) at 1013.0 hPa                                      |
| q) | Decomposition temperature                    | No data available                                                  |
| r) | Viscosity                                    | No data available                                                  |
| s) | Explosive properties                         | No data available                                                  |
| t) | Oxidizing properties                         | No data available                                                  |

## 9.2 Other safety information

|                        |                            |
|------------------------|----------------------------|
| Surface tension        | 22.8 mN/m at 25 °C (77 °F) |
| Relative vapor density | 4.91 - (Air = 1.0)         |

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heating.

### 10.5 Incompatible materials

Strong oxidizing agents, Strong reducing agents, Strong bases

## 10.6 Hazardous decomposition products

In the event of fire: see section 5

---

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Oral: No data available

LD50 Oral - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - > 14.5 mg/l

(OECD Test Guideline 403)

Dermal: 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

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

#### Germ cell mutagenicity

No data available

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

#### 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**

Repeated dose toxicity - Rat - male - Oral - NOAEL (No observed adverse effect level) - 2,000 mg/kg

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

---

**SECTION 12: Ecological information**

**12.1 Toxicity**

|                  |                                                                                                            |
|------------------|------------------------------------------------------------------------------------------------------------|
| Toxicity to fish | flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - 30 mg/l - 96 h<br>(OECD Test Guideline 203) |
|------------------|------------------------------------------------------------------------------------------------------------|

|                                                     |                                                                                                  |
|-----------------------------------------------------|--------------------------------------------------------------------------------------------------|
| Toxicity to daphnia and other aquatic invertebrates | Immobilization EC50 - Daphnia magna (Water flea) - 37.2 mg/l - 48 h<br>(OECD Test Guideline 202) |
|-----------------------------------------------------|--------------------------------------------------------------------------------------------------|

|                   |                                                                                                                        |
|-------------------|------------------------------------------------------------------------------------------------------------------------|
| Toxicity to algae | Growth inhibition EC50 - Pseudokirchneriella subcapitata (green algae) - 46.9 mg/l - 72 h<br>(OECD Test Guideline 201) |
|-------------------|------------------------------------------------------------------------------------------------------------------------|

**12.2 Persistence and degradability**

|                  |                                                                                                     |
|------------------|-----------------------------------------------------------------------------------------------------|
| Biodegradability | aerobic - Exposure time 20 d<br>Result: 88 % - Readily biodegradable.<br>(OECD Test Guideline 301D) |
|------------------|-----------------------------------------------------------------------------------------------------|

**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 Endocrine disrupting properties**

No data available

**12.7 Other adverse effects**

No data available

---

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

---

## SECTION 14: Transport information

#### DOT (US)

UN number: 1157    Class: 3    Packing group: III  
Proper shipping name: Diisobutyl ketone  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 1157    Class: 3    Packing group: III    EMS-No: F-E, S-D  
Proper shipping name: DIISOBUTYL KETONE

#### IATA

UN number: 1157    Class: 3    Packing group: III  
Proper shipping name: Diisobutyl ketone

---

## SECTION 15: Regulatory information

#### SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

#### 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

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

#### Massachusetts Right To Know Components

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

---

## SECTION 16: Other information

#### 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.4

Revision Date: 03/03/2022

Print Date: 05/28/2022