

## SAFETY DATA SHEET

Version 6.4  
Revision Date 02/25/2021  
Print Date 11/27/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2,6-Dimethyl-5-heptenal

Product Number : W238920

Brand : Aldrich

CAS-No. : 106-72-9

**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 4), H227

Skin sensitization (Sub-category 1B), H317

Short-term (acute) aquatic hazard (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



Signal word

Warning

Hazard statement(s)

H227

Combustible liquid.

H317	May cause an allergic skin reaction.
H401	Toxic to aquatic life.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P272	Contaminated work clothing must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
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	: Melonal Melon aldehyde
Formula	: C <sub>9</sub> H <sub>16</sub> O
Molecular weight	: 140.22 g/mol
CAS-No.	: 106-72-9
EC-No.	: 203-427-2

Component	Classification	Concentration
<b>2,6-Dimethyl-5-heptenal</b>	Flam. Liq. 4; Skin Sens. 1B; Aquatic Acute 2; H227, H317, H401	<= 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. Move out of dangerous area.

#### 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**

Do NOT induce vomiting. 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.

**Unsuitable extinguishing media**

Do NOT use water jet.

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

Carbon oxides  
Combustible.

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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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. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.  
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**

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). 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.

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

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

#### **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.

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**

Face shield and safety glasses 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**

Complete suit protecting against chemicals, 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<br>Color: colorless  |
| b) Odor   | No data available   |
| c) Odor Threshold                               | No data available   |
| d) pH   | No data available   |
| e) Melting point/freezing point                 | Freezing point: < -20 °C (< -4 °F) - OECD Test Guideline 102  |
| f) Initial boiling point and boiling range      | 181 °C 358 °F at 1,016 hPa - OECD Test Guideline 103  |
| g) Flash point                                  | 62 °C (144 °F) - Regulation (EC) No. 440/2008, Annex, A.9   |
| 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                               | 1.51 hPa at 20 °C (68 °F) - OECD Test Guideline 104<br>2.39 hPa at 25 °C(77 °F) - OECD Test Guideline 104 |
| l) Vapor density                                | No data available   |
| m) Relative density                             | 0.85 at 20 °C (68 °F) - OECD Test Guideline 109   |
| n) Water solubility                             | 0.5 g/l at 20 °C (68 °F) - OECD Test Guideline 105  |
| o) Partition coefficient: n-octanol/water       | log Pow: 3.4 at 35 °C (95 °F) - OECD Test Guideline 117 -<br>Bioaccumulation is not expected.             |
| p) Autoignition temperature                     | 208 °C (406 °F) at 1,012 - 1,021 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 | 52.9 mN/m at 0.46g/l at 20 °C (68 °F) - OECD Test Guideline 115 |
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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

Heat, flames and sparks.

### 10.5 Incompatible materials

Strong oxidizing agents, Strong bases

### 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 - > 5,000 mg/kg

Remarks:

(RTECS)

Inhalation: No data available

LD50 Dermal - Rabbit - > 5,000 mg/kg

Remarks:

(RTECS)

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

#### Germ cell mutagenicity

Ames test

Escherichia coli/Salmonella typhimurium

Result: negative

sister chromatid exchange assay

rat hepatocytes

Result: negative

OECD Test Guideline 474

Mouse - male and female - Bone marrow

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

### **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: MJ8797000

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**

No data available

Toxicity to daphnia and other aquatic invertebrates      semi-static test EC50 - Daphnia magna (Water flea) - 2.4 mg/l - 48 h  
(OECD Test Guideline 202)

Toxicity to bacteria      NOEC - activated sludge - 100 mg/l - 39 d

### **12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 28 d  
Result: 75 % - 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**

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.

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Contact a licensed professional waste disposal service to dispose of this material. Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

NA-Number: 1993 Class: NONE Packing group: III

Proper shipping name: Combustible liquid, n.o.s. (2,6-Dimethyl-5-heptenal)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

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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

Fire Hazard, Acute Health Hazard

### Massachusetts Right To Know Components

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



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## **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](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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