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: 109991
Brand: Aldrich
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

Aldrich - 109991
Hazard Statements
H226  Flammable liquid and vapor.
H335  May cause respiratory irritation.

Precautionary Statements
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

3.2 Mixtures
Synonyms:  Diisobutyl ketone
           Isovalerone

Formula:  C₉H₁₈O
Molecular weight:  142.24 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>2,6-Dimethylheptan-4-one</strong></td>
<td>Flam. Liq. 3; STOT SE 3;</td>
<td>&gt;= 50 - &lt; 70 %</td>
</tr>
<tr>
<td>CAS-No. 108-83-8</td>
<td>H226, H335</td>
<td></td>
</tr>
<tr>
<td>EC-No. 203-620-1</td>
<td>Concentration limits:</td>
<td></td>
</tr>
<tr>
<td>Index-No. 606-005-00-X</td>
<td>&gt;= 10 %: STOT SE 3, H335;</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>3,3,5-trimethylcyclohexanone</strong></td>
<td>Flam. Liq. 4; Eye Irrit. 2A;</td>
<td>&gt;= 1 - &lt; 5 %</td>
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<tr>
<td>CAS-No. 873-94-9</td>
<td>STOT SE 3; H227, H319, H335</td>
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</tr>
<tr>
<td>EC-No. 212-855-9</td>
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</tr>
</tbody>
</table>

Aldrich - 109991
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 (CO2) 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
<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
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</thead>
<tbody>
<tr>
<td>2,6-Dimethylheptan-4-one</td>
<td>108-83-8</td>
<td>TWA</td>
<td>25 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>25 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td>TWA</td>
<td>50 ppm</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>25 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>150 mg/m3</td>
<td></td>
</tr>
</tbody>
</table>

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
Recommended Filter type: Filter type ABEK
The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.
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: liquid
b) Odor No data available
c) Odor Threshold No data available
d) pH  
No data available

e) Melting point/freezing point  
No data available

f) Initial boiling point and boiling range  
165 - 170 °C 329 - 338 °F - lit.

g) Flash point  
49 °C (120 °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  
0.808 g/mL at 25 °C (77 °F) - lit.

Relative density  
No data available

n) Water solubility  
No data available

o) Partition coefficient: n-octanol/water  
No data available

p) Autoignition temperature  
No data available

q) Decomposition temperature  
No data available

r) Viscosity  
No data available

s) Explosive properties  
Not classified as explosive.

t) Oxidizing properties  
none

9.2 Other safety information  
No data available

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 bases, Strong oxidizing agents, Strong acids, Strong reducing agents

10.6 **Hazardous decomposition products**
In the event of fire: see section 5

---

**SECTION 11: Toxicological information**

11.1 **Information on toxicological effects**

**Mixture**

**Acute toxicity**
Oral: No data available
Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
Dermal: No data available

**Skin corrosion/irritation**
No data available

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
No data available

**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**
Mixture may cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
No data available

11.2 **Additional Information**
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.
Stomach - Irregularities - Based on Human Evidence

Components

2,6-Dimethylheptan-4-one

**Acute toxicity**
- 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)
- 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 sensitzation**
- 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
  - Result: negative

**Carcinogenicity**
- No data available

**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
3,3,5-trimethylcyclohexanone

**Acute toxicity**
LD50 Oral - Rat - male and female - > 2,000 mg/kg (OECD Test Guideline 401)
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
LC50 Inhalation - Rat - male - 4 h - 14.2 mg/l - aerosol (OECD Test Guideline 403)
Symptoms: Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract
Inhalation: absorption
LD50 Dermal - Rat - male and female - > 2,000 mg/kg (OECD Test Guideline 402)

**Skin corrosion/irritation**
Skin - Rabbit
Result: No skin irritation (OECD Test Guideline 404)

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
Buehler Test - Guinea pig
Result: negative (OECD Test Guideline 406)

**Germ cell mutagenicity**
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster lung cells
Result: negative
Method: OECD Test Guideline 474
Species: Mouse - male and female
Result: negative

**Carcinogenicity**
No data available

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
May cause respiratory irritation.
Acute oral toxicity - Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Acute inhalation toxicity - Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract

**Specific target organ toxicity - repeated exposure**
No data available
SECTION 12: Ecological information

12.1 Toxicity

**Mixture**
No data available

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 Endocrine disrupting properties
No data available

12.7 Other adverse effects
No data available

**Components**

**2,6-Dimethylheptan-4-one**

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

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

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

**3,3,5-trimethylcyclohexanone**

Toxicity to fish
static test LC50 - Danio rerio (zebra fish) - > 100 mg/l - 96 h
(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates
static test EC50 - Daphnia magna (Water flea) - 180 mg/l - 48 h
(OECD Test Guideline 202)

Toxicity to algae
static test ErC50 - Desmodesmus subspicatus (green algae) - > 82.27 mg/l - 72 h
(OECD Test Guideline 201)
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 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
Proper shipping name: DIISOBUTYL KETONE
EMS-No: F-E, S-D

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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,6-Dimethylheptan-4-one</td>
<td>108-83-8</td>
<td>1993-02-16</td>
</tr>
</tbody>
</table>

### Pennsylvania Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
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<tbody>
<tr>
<td>2,6-Dimethylheptan-4-one</td>
<td>108-83-8</td>
<td>1993-02-16</td>
</tr>
</tbody>
</table>

---

### SECTION 16: Other information

**Further information**
The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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.

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