SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 4-Heptanone

Product Number : W254606
Brand : Aldrich
Index-No. : 606-027-00-X
CAS-No. : 123-19-3

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
Acute toxicity, Inhalation (Category 4), H332

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.
H332 Harmful if inhaled.

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 mist or vapors.
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 + 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

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>Butyrone</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Dipropyl ketone</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₇H₁₄O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>114.19 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>123-19-3</td>
</tr>
<tr>
<td>EC-No.</td>
<td>204-608-9</td>
</tr>
<tr>
<td>Index-No.</td>
<td>606-027-00-X</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-heptanone</td>
<td>Flam. Liq. 3; Acute Tox. 4;</td>
<td>&lt;= 100 %</td>
</tr>
<tr>
<td></td>
<td>H226, H332</td>
<td></td>
</tr>
</tbody>
</table>

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. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

**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: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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**
Carbon dioxide (CO2) Foam 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 safe handling
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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. Preventive skin protection recommended. 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
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-heptanone</td>
<td>123-19-3</td>
<td>TWA</td>
<td>50 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>50 ppm 235 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>50 ppm 235 mg/m³</td>
<td>California permissible exposure limits</td>
</tr>
</tbody>
</table>

### 8.2 Exposure controls

**Appropriate engineering controls**
Change contaminated clothing. Preventive skin protection recommended. 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**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 60 min
Material tested: Butoject® (KCL 898)

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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
   Melting point/range: -33 °C (-27 °F) - lit.
f) Initial boiling point and boiling range
   145 °C 293 °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
   6.9 hPa at 20 °C (68 °F)
l) Vapor density
   3.94 - (Air = 1.0)
m) Density
   0.817 g/cm3 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
   No data available
t) Oxidizing properties
   none

9.2 Other safety information

Relative vapor density
3.94 - (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
increased reactivity with:
Strong oxidizing agents
strong reducing agents
Strong bases

10.4 Conditions to avoid
Heating.

10.5 Incompatible materials
Strong oxidizing agents

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
LD50 Oral - Rat - 3,730 mg/kg
Remarks: (RTECS)
LC50 Inhalation - Rat - 4 h - 14.42 mg/l - vapor
Remarks: (RTECS)
LD50 Dermal - Rabbit - 5,660 mg/kg
Remarks: (RTECS)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
Remarks: (RTECS)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
Remarks: (RTECS)

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**
No data available

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

**Aspiration hazard**
No data available

### 11.2 Additional Information

RTECS: MJ5600000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

The following applies to ketones in general: when vapours/aerosols occur, mucosal irritations, coughing, and dyspnœa after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

Further data:

Handle in accordance with good industrial hygiene and safety practice.

### SECTION 12: Ecological information

12.1 **Toxicity**
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
We have no quantitative data concerning the ecological effects of this product.
Further information on ecology
Discharge into the environment must be avoided.

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.

SECTION 14: Transport information
DOT (US)
UN number: 2710  Class: 3  Packing group: III
Proper shipping name: Dipropyl ketone
Reportable Quantity (RQ): Poison Inhalation Hazard: No

IMDG
UN number: 2710  Class: 3  Packing group: III  EMS-No: F-E, S-D
Proper shipping name: DIPROPYL KETONE

IATA
UN number: 2710  Class: 3  Packing group: III
Proper shipping name: Dipropyl 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

Massachusetts Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-heptanone</td>
<td>123-19-3</td>
<td>1993-02-16</td>
</tr>
</tbody>
</table>

Pennsylvania Right To Know Components

Aldrich - W254606
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.

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Version: 6.5 Revision Date: 08/27/2023 Print Date: 01/11/2024