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

1.1 Product identifiers

Product name: Heptane

Product Number: 154873
Brand: Sigma-Aldrich
Index-No.: 601-008-00-2
CAS-No.: 142-82-5

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 2), H225
Skin irritation (Category 2), H315
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

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: Danger

Hazard statement(s):
- H225: Highly flammable liquid and vapor.
- H304: May be fatal if swallowed and enters airways.
- H315: Causes skin irritation.
- H336: May cause drowsiness or dizziness.
- H410: Very toxic to aquatic life with long lasting effects.

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.
- P264: Wash skin thoroughly after handling.
- P271: Use only outdoors or in a well-ventilated area.
- P273: Avoid release to the environment.
- P280: Wear protective gloves/ eye protection/ face protection.
- P301 + P310: IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
- 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.
- P331: Do NOT induce vomiting.
- P332 + P313: If skin irritation occurs: Get medical advice/ attention.
- P362: Take off contaminated clothing and wash before reuse.
- P370 + P378: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- P391: Collect spillage.
- 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

<table>
<thead>
<tr>
<th>Formula</th>
<th>C\textsubscript{7}H\textsubscript{16}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>100.20 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>142-82-5</td>
</tr>
<tr>
<td>EC-No.</td>
<td>205-563-8</td>
</tr>
<tr>
<td>Index-No.</td>
<td>601-008-00-2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-heptane</td>
<td>Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1;</td>
<td>&lt;= 100 %</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. 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

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
Flash back possible over considerable distance.
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.
5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **Further information**
In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion. 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 carefully 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_
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

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

_Storage conditions_
Store under inert gas. 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>
</tr>
</thead>
<tbody>
<tr>
<td>n-heptane</td>
<td>142-82-5</td>
<td>TWA</td>
<td>85 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>350 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>C</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>440 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1,800 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>500 ppm</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2,000 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>400 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1,600 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>500 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2,000 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>400 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>STEL</td>
<td>500 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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
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.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.2 mm
Break through time: 65 min
Material tested: Dermatril® P (KCL 743 / Aldrich Z677388, Size M)
data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

**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.

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**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: liquid</td>
</tr>
<tr>
<td>b) Odor</td>
<td>No data available</td>
</tr>
<tr>
<td>c) Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>Melting point/range: -91 °C (-132 °F)</td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>98 °C 208 °F</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>-4 °C (25 °F) - c.c.</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
</tbody>
</table>
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 7 %(V)  
                                          | Lower explosion limit: 1.1 %(V) |
| k) Vapor pressure                       | 48 hPa at 20.0 °C (68.0 °F)  |
| l) Vapor density                        | No data available            |
| m) Density                              | 0.684 g/mL at 25 °C (77 °F)  |
| Relative density                        | No data available            |
n) Water solubility: insoluble
o) Partition coefficient: log Pow: > 3 - Bioaccumulation is not expected.

SECTION 10: Stability and reactivity

10.1 Reactivity
Vapors may form explosive mixture with air.

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

10.3 Possibility of hazardous reactions
Risk of ignition or formation of inflammable gases or vapours with:
- Strong oxidizing agents: phosphorus
  in the presence of: Chlorine

10.4 Conditions to avoid
Warming.

10.5 Incompatible materials
rubber, various plastics

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 - male and female - > 5,000 mg/kg
(OECD Test Guideline 401)
Remarks: (in analogy to similar compounds)
The value is given in analogy to the following substances: isooctane
LC50 Inhalation - Rat - male and female - 4 h - > 29.29 mg/l - vapor
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

Remarks: The value is given in analogy to the following substances: isoctane

**Skin corrosion/irritation**

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: The value is given in analogy to the following substances: isoctane

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

Remarks: The value is given in analogy to the following substances: isoctane

**Respiratory or skin sensitization**

Maximization Test - Guinea pig

Result: negative

Remarks: Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: rat hepatocytes

Method: OECD Test Guideline 473

Result: negative

**Carcinogenicity**

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

May cause drowsiness or dizziness.

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

May be fatal if swallowed and enters airways.

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.
11.2 Additional Information

RTECS: MI7700000
Prolonged or repeated exposure to skin causes defatting and dermatitis., Central nervous system depression, narcosis, Damage to the lungs.
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
No data available

12.2 Persistence and degradability

<table>
<thead>
<tr>
<th>Biodegradability</th>
<th>aerobic - Exposure time 10 d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Result</td>
<td>70 % - Readily biodegradable.</td>
</tr>
<tr>
<td>Remarks</td>
<td>(ECHA)</td>
</tr>
</tbody>
</table>

Biochemical Oxygen Demand (BOD) 1,920 mg/g
Remarks: (IUCLID)

Theoretical oxygen demand 3,500 mg/g
Remarks: (Lit.)

Ratio BOD/ThBOD 55 %
Remarks: (Lit.)

12.3 Bioaccumulative potential
Indication of bioaccumulation.

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
Additional ecological information
Do not empty into drains. Avoid release to the environment.

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: 1206
- Class: 3
- Packing group: II
- Proper shipping name: Heptanes
- Marine pollutant: yes
- Poison Inhalation Hazard: No

**IMDG**
- UN number: 1206
- Class: 3
- Packing group: II
- EMS-No: F-E, S-D
- Proper shipping name: HEPTANES
- Marine pollutant: yes

**IATA**
- UN number: 1206
- Class: 3
- Packing group: II
- Proper shipping name: Heptanes

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>n-heptane</td>
<td>142-82-5</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>
</thead>
<tbody>
<tr>
<td>n-heptane</td>
<td>142-82-5</td>
<td>1993-02-16</td>
</tr>
</tbody>
</table>

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
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Version: 6.6  Revision Date: 03/18/2023  Print Date: 07/30/2023