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

Sigma-Aldrich - 154873
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>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>

Formula : C\textsubscript{7}H\textsubscript{16}
Molecular weight : 100.20 g/mol
CAS-No. : 142-82-5
EC-No. : 205-563-8
Index-No. : 601-008-00-2

Sigma-Aldrich - 154873
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></td>
<td>TWA</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>500 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2,000 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>PEL</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>400 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1,600 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>STEL</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>500 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2,000 mg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>400 ppm</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>STEL</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>500 ppm</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)
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>a) Appearance</th>
<th>Form: liquid</th>
</tr>
</thead>
<tbody>
<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>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>Upper explosion limit: 7 % (V) Lower explosion limit: 1.1 % (V)</td>
</tr>
<tr>
<td>k) Vapor pressure</td>
<td>48 hPa at 20.0 °C (68.0 °F)</td>
</tr>
<tr>
<td>l) Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td>m) Density</td>
<td>0.684 g/mL at 25 °C (77 °F)</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
</tbody>
</table>
n) Water solubility        insoluble
o) Partition coefficient: n-octanol/water  log Pow: > 3 - Bioaccumulation is not expected.
p) Autoignition temperature 223.0 °C (433.4 °F)
q) Decomposition temperature No data available
r) Viscosity 0.64 mm²/s at 20 °C (68 °F)
s) Explosive properties No data available
t) Oxidizing properties none

9.2 Other safety information
No data available

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: isoctane
     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.

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**
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
Biodegradability
- aerobic: Exposure time 10 d
  Result: 70 % - Readily biodegradable.
  Remarks: (ECHA)

  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)**

<table>
<thead>
<tr>
<th>UN number: 1206</th>
<th>Class: 3</th>
<th>Packing group: II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proper shipping name: Heptanes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reportable Quantity (RQ):</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Marine pollutant: yes</td>
<td>Poison Inhalation Hazard: No</td>
<td></td>
</tr>
</tbody>
</table>

**IMDG**

<table>
<thead>
<tr>
<th>UN number: 1206</th>
<th>Class: 3</th>
<th>Packing group: II</th>
<th>EMS-No: F-E, S-D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proper shipping name: HEPTANES</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Marine pollutant: yes</td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

**IATA**

<table>
<thead>
<tr>
<th>UN number: 1206</th>
<th>Class: 3</th>
<th>Packing group: II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proper shipping name: Heptanes</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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>n-heptane</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>142-82-5</td>
<td>1993-02-16</td>
<td></td>
</tr>
</tbody>
</table>

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>n-heptane</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>142-82-5</td>
<td>1993-02-16</td>
<td></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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product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.6           Revision Date: 03/18/2023           Print Date: 10/22/2023