

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**Product name : Heptane-1-¹³CProduct Number : 492728
Brand : Aldrich

CAS-No. : 75560-45-1

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 sheetCompany : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USATelephone : +1 800-325-5832
Fax : +1 800-325-5052**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (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 vapour.

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/ vapours/ 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/ protective clothing/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P312	Call a POISON CENTER/doctor if you feel unwell.
P321	Specific treatment (see supplemental first aid instructions on this label).
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 for extinction.
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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula	: $^{13}\text{CC}_6\text{H}_{16}$
Molecular weight	: 101.19 g/mol
CAS-No.	: 75560-45-1

Hazardous components

Component	Classification	Concentration
Heptane-1-13C		
	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H304, H315, H336, H410	90 - 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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

5. FIREFIGHTING MEASURES**5.1 Extinguishing media****Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

No data available

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.

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours 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 an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Heptane-1-13C	75560-45-1	TWA	500 ppm 2,000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
	Remarks	The value in mg/m3 is approximate.		
		TWA	500.000000 ppm 2,000.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	400 ppm 1,600 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	500 ppm 2,000 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	400.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		TWA	400 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		STEL	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		STEL	500.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		TWA	85.000000 ppm 350.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		C	440.000000 ppm 1,800.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		15 minute ceiling value		
		TWA	400.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		STEL	500.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		TWA	400 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		

		STEL	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation		
		PEL	400 ppm 1,600 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	500 ppm 2,000 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

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, Flame retardant antistatic protective clothing., 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|--|
| a) Appearance | Form: liquid |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: -91 °C (-132 °F) - lit. |
| f) Initial boiling point and boiling range | 98 °C (208 °F) - lit. |
| g) Flash point | -4.00 °C (24.80 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 7.00 %(V)
Lower explosion limit: 1.10 %(V) |

k) Vapour pressure	111 hPa (83 mmHg) at 37.70 °C (99.86 °F) 53 hPa (40 mmHg) at 20.00 °C (68.00 °F)
l) Vapour density	No data available
m) Relative density	0.691 g/mL at 25 °C (77 °F) 0.691 g/cm ³ at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	log Pow: > 3.000
p) Auto-ignition temperature	No data available
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

No data available

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

Vapours may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: Irritating to respiratory system.

LC50 Inhalation - Rat - 4.00 h - 103,000 mg/m³

Dermal: No data available

LD50 Intravenous - Mouse - 222 mg/kg

No data available

No data available

Skin corrosion/irritation

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

- IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- NTP: No component 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

No data available

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

Additional Information

RTECS: Not available

Exposure to large amounts can cause:, Nausea, Dizziness, Headache, narcosis

12. ECOLOGICAL INFORMATION**12.1 Toxicity****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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Very toxic to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1206 Class: 3 Packing group: II
Proper shipping name: Heptanes
Reportable Quantity (RQ): 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 Marine pollutant: yes

IATA

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

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.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Heptane-1-13C	75560-45-1	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Heptane-1-13C	75560-45-1	1993-04-24

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Asp. Tox.	Aspiration hazard
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
Skin Irrit.	Skin irritation

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	3

Physical Hazard 0

NFPA Rating

Health hazard: 2

Fire Hazard: 3

Reactivity Hazard: 0

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation

Product Safety – Americas Region

1-800-521-8956

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