

SAFETY DATA SHEET

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

1.1 Product identifiers

Product name n-Heptane
CAS number 142-82-5
Synonyms Heptane

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 Lab Alley, LLC
 12501 Pauls Valley Road
 Austin, Texas 78737
 U.S.A.

Telephone 512-668-9918
Fax 512-886-4008

1.4 Emergency telephone

Emergency Phone # US & Canada: 1-800-535-5053 INFOTRAC
 International 1-352-323-3500 INFOTRAC


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)
Skin irritation (Category 2)
Specific target organ toxicity - single exposure (Category 3)
Target organ - Central nervous system (CNS)
Aspiration hazard (Category 1)
Short-term (acute) aquatic hazard (Category 1)
Long-term (chronic) aquatic hazard (Category 1)

2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal Word	Danger
Hazard statements	Highly flammable liquid and vapor. May be fatal if swallowed and enters airways. Causes skin irritation. May cause drowsiness or dizziness. Very toxic to aquatic life with long lasting effects.
Precautionary statements	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking. Keep container tightly closed. Ground/bond container and receiving equipment. Use explosion-proof electrical/ ventilating/ lighting/ equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray. Wash skin thoroughly after handling. Use only outdoors or in a well-ventilated area. Avoid release to the environment. Wear protective gloves/ eye protection/ face protection. IF SWALLOWED: Immediately call a POISON CENTER/ doctor. IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell. Do NOT induce vomiting. If skin irritation occurs: Get medical advice/ attention. Take off contaminated clothing and wash before reuse.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

None.

SECTION 3: Composition/information on ingredients

3.1 Components

Chemical name	Common name and synonyms	CAS number	Concentration
n-Heptane	N/A	142-82-5	> 99%
Methylcyclohexane	N/A	108-87-2	0 - 0.2%
Isooctane	N/A	26635-64-3	0 - 0.1%
Dimethylcyclopentane	N/A	28729-52-4	0 - 0.1%

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

If inhaled	Move to fresh air. If breathing is difficult, give oxygen. Obtain medical attention. Aspiration into lungs can produce severe lung damage.
In case of skin contact	Take off immediately all contaminated clothing. Wash off immediately with plenty of water for at least 15 minutes. Obtain medical attention.
In case of eye contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Obtain medical attention.
If swallowed	Do not induce vomiting. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician or Poison Control Center immediately.

4.2 Most important symptoms and effects, both acute and delayed

Breathing difficulties. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting. 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 information available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media	Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray. Water may be ineffective.
Unsuitable extinguishing media	No information available.

5.2 Specific hazards arising from the substance or mixture

Flammable. Risk of ignition. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Do not allow run-off from fire fighting to enter drains or water courses.

5.3 Special protective equipment and precautions for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

5.4 Further information

Flash Point -4 °C / 25 °F

Autoignition Temperature 223.0 °C / 433.4 °F

Explosion limits

Upper 7% (V)

Lower 1.1% (V)

Sensitivity to Mechanical Impact No information available.

Sensitivity to Static Discharge No information available.

NFPA

Health	Flammability	Instability	Physical hazards
3	3	0	N/A

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 flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained. See Section 12 for additional ecological information. Avoid release to the environment. Collect spillage.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges. Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

See Section 2 for full list of hazard and precaution statements.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Precautions on safe handling

Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Ensure adequate ventilation. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges. Use explosion-proof equipment.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Store under inert gas. Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat and sources of ignition. Flammables area. Storage class (TRGS 510): 3: Flammables liquids.

Incompatibilities

Strong oxidizing agents. Rubber, various plastics.

SECTION 8: Exposure controls/personal protection

8.1 Occupational exposure limits

US. OSHA Table Z-1 Limits for Air Contaminants (29 CFR 1910.1000)

Component	Type	Value	
n-heptane	TWA	500 ppm	2000 mg/m ³
Methylcyclohexane	TWA	500 ppm	2000 mg/m ³

US. ACGIH Threshold Limit Values

Component	Type	Value	
n-heptane	STEL	500 ppm	
	TWA	400 ppm	
Methylcyclohexane	TWA	400 ppm	
Isooctane	TWA	300 ppm	

US. NIOSH: Pocket Guide to Chemical Hazards

Component	Type	Value	
n-heptane	IDLH	750 ppm	
	TWA	85 ppm	350 mg/m ³
	Ceiling	440 ppm	1800 mg/m ³
Methylcyclohexane	IDLH	1200 ppm	
	TWA	400 ppm	1600 mg/m ³

Biological occupational exposure limits

No information available.

8.2 Exposure controls

Appropriate engineering controls

Use only under a chemical fume hood. Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting/equipment. Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166. Tightly fitting safety goggles. Face-shield.

Skin protection

Wear appropriate protective gloves.

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. Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

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

Physical State	Liquid
Appearance	Colorless
Odor	Petroleum Distillates
Odor Threshold	No information available.
pH	No information available.
Melting Point/Range	-91 °C / -132 °F
Boiling Point/Range	98 °C / 208 °F
Evaporation Rate	No information available.
Flammability (solid)	Not applicable.
Flammability or explosive limit	
Upper	7% (V)
Lower	1.1% (V)
Vapor Pressure	111 hPa at 37.7 °C / 99.9 °F 53.3 hPa at 20.0 °C / 68.0 °F

Vapor Density	No information available.
Density	0.684 g/mL at 25 °C / 77 °F
Solubility	Insoluble
Partition coefficient; n-octanol/water	No information available.
Autoignition Temp	223.0 °C / 433.4 °F
Decomposition Temp	No information available.
Viscosity	0.64 mm ² /s at 20 °C / 68 °F
Molecular Formula	C ₇ H ₁₆
Molecular Weight	100.20 g/mol
VOC Content(%)	No information available.
Oxidizing properties	None.

9.2 Other safety information

No information available.

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture in air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

None under normal processing.

10.4 Conditions to avoid

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.

10.5 Incompatible materials

Strong oxidizing agents. Rubber, various plastics.

10.6 Hazardous decomposition products

Carbon monoxide (CO), Carbon dioxide (CO₂).

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Product Information, Component Information

Acute toxicity

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
n-Heptane	> 2000 mg/kg (rat)	3000 mg/kg (rabbit)	103 g/m ³ (rat)
Methylcyclohexane	3200 mg/kg (rat)	86700 mg/kg (rabbit)	Not listed.

Skin corrosion/irritation

Irritating to skin.

Serious eye damage/eye irritation

Irritating to eyes.

Respiratory or skin sensitization

No information available.

Germ cell mutagenicity

No information available.

Carcinogenicity

Component	CAS	IARC	NTP	ACGIH	OSHA	Mexico
n-Heptane	142-82-5	Not listed	Not listed	Not listed	Not listed	Not listed
Methylcyclohexane	108-87-2	Not listed	Not listed	Not listed	Not listed	Not listed
Isooctane	26635-64-3	Not listed	Not listed	Not listed	Not listed	Not listed
Dimethylcyclopentane	28729-52-4	Not listed	Not listed	Not listed	Not listed	Not listed

Specific target organ toxicity - single exposure

Respiratory system, Central nervous system (CNS)

Specific target organ toxicity - repeated exposure

None known.

Reproductive toxicity

No information available.

Chronic effects

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

11.2 Additional Information

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.

SECTION 12: Ecological information**12.1 Toxicity**

Product		Species	Test Results
n-Heptane	LC50	Freshwater fish	375.0 mg/L 96 h
	EC50	Water flea	> 10 mg/L 24 h

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 Bio accumulative potential

Indication of bioaccumulation.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

No information available.

12.6 Endocrine disrupting properties

No information available.

12.7 Other adverse effects

Do not empty into drains. Avoid release to the environment.

SECTION 13: Disposal considerations

13.1 Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

SECTION 14: Transport information

DOT (US)

UN-no	UN1206
Proper Shipping Name	Heptanes
Hazard Class	3
Packing Group	II

IMDG

UN-no	UN1206
Proper Shipping Name	Heptanes
Hazard Class	3
Packing Group	II

IATA

UN-no	UN1206
Proper Shipping Name	Heptanes
Hazard Class	3

SECTION 15: Regulatory information

US federal regulations This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not listed.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not regulated.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous

Acute Health Hazard
Chronic Health Hazard
Fire Hazard

SARA 313 (TRI reporting)

Not regulated.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act

Not regulated.

FEMA Priority Substances Respiratory Health and Safety in the Flavor Manufacturing Workplace

Not listed.

US state regulations

US. Massachusetts RTK - Substance List

Listed. (n-Heptane and Methylcyclohexane)

US. New Jersey Worker and Community Right-to-Know Act

Listed. (n-Heptane and Methylcyclohexane)

US. Pennsylvania Worker and Community Right-to-Know Law

Listed. (n-Heptane, Methylcyclohexane, and Isooctane)

California Proposition 65

Not listed.

SECTION 16: Other information

Issue date: 03/07/2017

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Revision 2: 10/02/2024

SECTION 17: Disclaimer

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.