

## 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; Normal Heptane; Ligroine; Petroleum Ether

#### 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  
22111 Highway 71 West, Suite 601  
Spicewood, Texas 78669  
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), Central nervous system  
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 statement(s):

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 statement(s):

**Prevention** - 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.  
**Response** - 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. Rake off contaminated clothing and wash before reuse.

**Hazards not otherwise classified**

None.

## SECTION 3: Composition/information on ingredients

### 3.1 Components

Component	CAS-No	Weight %
n-Heptane	142-82-5	>99
Methylcyclohexane	108-87-2	0 - 0.2
Isooctane	26635-64-3	0 - 0.1
Dimethylcyclopentane	28729-52-4	0 - 0.1

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

**General advice:**

Show this safety data sheet to the doctor in attendance.

**If inhaled:**

Move to fresh air. If breathing is difficult, give oxygen. Obtain medical attention. Aspiration into lungs can produce severe lung damage.

<b>In case of skin contact:</b>	Take off immediately all contaminated clothing. Wash off immediately with plenty of water for at least 15 minutes. Obtain medical attention.
<b>In case of eye contact:</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Obtain medical attention.
<b>If swallowed:</b>	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 data available.

# SECTION 5: Firefighting measures

## 5.1 Extinguishing media

### Suitable (and unsuitable) 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.

## 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

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 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

For disposal see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for 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

Immediately change contaminated clothing. Apply preventative 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 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.

## 8. Exposure controls/personal protection

### 8.1 Occupational exposure limits

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH
n-Heptane	TWA: 400 ppm STEL: 500 ppm	(Vacated) TWA: 400 ppm (Vacated) TWA: 1600 mg/m <sup>3</sup> (Vacated) STEL: 500 ppm (Vacated) STEL: 2000 mg/m <sup>3</sup> TWA: 500 ppm TWA: 2000 mg/m <sup>3</sup>	IDLH: 750 ppm TWA: 85 ppm TWA: 350 mg/m <sup>3</sup> Ceiling: 440 ppm Ceiling: 1800 mg/m <sup>3</sup>
Methylcyclohexane	TWA: 400 ppm	(Vacated) TWA: 400 ppm (Vacated) TWA: 1600 mg/m <sup>3</sup> TWA: 500 ppm TWA: 2000 mg/m <sup>3</sup>	IDLH: 1200 ppm TWA: 400 ppm TWA: 1600 mg/m <sup>3</sup>
Isooctane	TWA: 300 ppm		

Component	Quebec	Mexico OEL (TWA)	Ontario TWAEV
n-Heptane	TWA: 400 ppm TWA: 1640 mg/m <sup>3</sup> STEL: 500 ppm STEL: 2050 mg/m <sup>3</sup>	TWA: 400 ppm TWA: 1600 mg/m <sup>3</sup> STEL: 500 ppm STEL: 2000 mg/m <sup>3</sup>	TWA: 400 ppm STEL: 500 ppm
Methylcyclohexane	TWA: 400 ppm TWA: 1610 mg/m <sup>3</sup>	TWA: 400 ppm TWA: 1600 mg/m <sup>3</sup> STEL: 500 ppm STEL: 2000 mg/m <sup>3</sup>	TWA: 400 ppm

## 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 and body protection

Flame retardant antistatic protective clothing. Long sleeved 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

<b>Physical State</b>	Liquid.
<b>Appearance</b>	Colorless.
<b>Odor</b>	Petroleum Distillates
<b>Odor Thresh</b>	No data available.
<b>pH</b>	No data available.
<b>Melting Point/Range</b>	-91 °C (-132 °F)
<b>Boiling Point/Range</b>	98 °C 208 °F
<b>Flash Point</b>	-4 °C (25 °F) - c.c.
<b>Evaporation Rate</b>	No data available.
<b>Flammability (solid, gas)</b>	No data available.
<b>Flammability or explosive limit</b>	
	<b>Upper</b> : 7% (V)
	<b>Lower</b> : 1.1% (V)

<b>Vapor Pressure</b>	111 hPa at 37.7 °C (99.9 °F) 53.3 hPa at 20.0 °C(68.0 °F)
<b>Vapor Density</b>	No data available.
<b>Density</b>	0.684 g/mL at 25 °C (77 °F)
<b>Solubility</b>	Insoluble
<b>Partition coefficient; n-octanol/water</b>	log Pow: > 3 - Bioaccumulation is not expected.
<b>Autoignition Temp</b>	223.0 °C (433.4 °F)
<b>Decomposition Temp</b>	No data available.
<b>Viscosity</b>	0.64 mm <sup>2</sup> /s at 20 °C (68 °F)
<b>Molecular Formula</b>	C <sub>7</sub> H <sub>16</sub>
<b>Molecular Weight</b>	100.20 g/mol
<b>VOC Content(%)</b>	No data available.
<b>Oxidizing properties</b>	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

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 (CO<sub>2</sub>).

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute Toxicity

#### Product Information

#### Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
n-Heptane	>2000 mg/kg (rat)	3000 mg/kg ( Rabbit )	103 g/m <sup>3</sup> ( Rat ) 4 h
Methylcyclohexane	3200 mg/kg ( Rat )	86700 mg/kg ( Rabbit )	Not listed

**Toxicologically Synergistic** No information available

#### Products

#### Delayed and immediate effects as well as chronic effects from short and long-term exposure

**Irritation** Irritating to eyes and skin

**Sensitization** No information available

**Carcinogenicity** The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	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

**Mutagenic Effects** No information available

**Reproductive Effects** No information available.

**Developmental Effects** No information available.

**Teratogenicity** No information available.

**STOT - single exposure** Respiratory system Central nervous system (CNS)

**STOT - repeated exposure** None known

**Aspiration hazard** No information available

**Symptoms / effects, both acute and delayed** 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

**Other Adverse Effects** The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information.

### 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.

## 12. Ecological information

### 12.1 Toxicity

#### Ecotoxicity

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
n-Heptane	Not listed	375.0 mg/L LC50 96 h	Not listed	EC50: >10 mg/L/24h

### 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 information available.

### 12.7 Other adverse effects

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

## 13. Disposal considerations

### 13.1 Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. 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: 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

## SECTION 15: Regulatory information

### International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
n-Heptane	X	X	-	205-563-8	-		X	X	X	X	X
Methylcyclohexane	X	X	-	203-624-3	-		X	X	X	X	X
Isooctane	X	-	X	247-861-0	-		X	X	-	X	X
Dimethylcyclopentane	-	-	-	249-193-5	-		-	-	-	X	-

#### Legend:

X - Listed

E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.

F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.

N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.

P - Indicates a commenced PMN substance

R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.

S - Indicates a substance that is identified in a proposed or final Significant New Use Rule

T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.

XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B)).

Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.

Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

### U.S. Federal Regulations

TSCA 12(b)

SARA 313

Not applicable

**SARA 311/312 Hazardous Categorization**

Acute Health Hazard	Yes
Chronic Health Hazard	Yes
Fire Hazard	Yes
Sudden Release of Pressure Hazard	No
Reactive Hazard	No

**Clean Water Act** Not applicable

**Clean Air Act** Not applicable

**OSHA** Occupational Safety and Health Administration  
Not applicable

**CERCLA**

Not applicable

**California Proposition 65** This product does not contain any Proposition 65 chemicals

**State Right-to-Know**

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
n-Heptane	X	X	X	-	X
Methylcyclohexane	X	X	X	-	X
Isooctane	-	-	X	-	-

**U.S. Department of Transportation**

Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

**U.S. Department of Homeland Security**

This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** Serious risk, Grade 3

**Canada**

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations (CPR) and the MSDS contains all the information required by the CPR

**WHMIS Hazard Class** B2 Flammable liquid  
D2B Toxic materials



## SECTION 16: Other information

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**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.