

SAFETY DATA SHEET

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

1.1 Product identifiers

Product name	Heptane
CAS number	142-82-5
Synonyms	Normal heptane; Dipropylmethane

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Laboratory chemicals.
-----------------	-----------------------

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 Target Organ(s) - Central nervous system (CNS)	Category 3
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

Prevention: Wash face, hands, and any exposed skin thoroughly after handling. Wear protective gloves/protective clothing/eye protection/face protection Do not breathe dust/fume/gas/mist/vapors/spray. Use only outdoors or in a well-ventilated area. 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. Keep cool. Avoid release to the environment.

Response: Get medical attention/advice if you feel unwell.

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician if you feel unwell.

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. Wash contaminated clothing before reuse. If skin irritation occurs: Get medical advice/attention.

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. Do NOT induce vomiting.

Fire: In case of fire, use CO₂, dry chemical, or foam for extinction.

Storage: Store locked up. Store in a well-ventilated place. Keep container tightly closed.

Disposal: Dispose of contents/container to an approved waste disposal plant.

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

None identified.

SECTION 3: Composition/information on ingredients

3.1 Components

Chemical name	Common name and synonyms	CAS number	Concentration
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

If inhaled	Remove to fresh air. Get medical attention. Aspiration into lungs can produce severe lung damage. If not breathing, give artificial respiration. Risk of serious damage to the lungs (by aspiration).
In case of skin contact	Wash off immediately with plenty of water for at least 15 minutes. Get medical attention.
In case of eye contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
If swallowed	Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.

4.2 Most important symptoms and effects, both acute and delayed

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea, and vomiting.

4.3 Indication of any immediate medical attention and special treatment needed

If symptoms persist, call a physician. Treat symptomatically.

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam. Water mist maybe used to cool closed containers.

Unsuitable extinguishing media 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.

Hazardous Combustion Products: Carbon monoxide (CO). Carbon dioxide (CO₂).

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) - c.c.

Autoignition Temperature 223.0 °C (433.4 °F)

Explosion limits

Upper 7%

Lower 1.10%

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

Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

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.

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.

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/face protection. 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 spark-proof tools and 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

Keep containers tightly closed in a dry, cool, and well-ventilated place. Keep away from heat, sparks, and flame. Flammables area.

Incompatibilities

Strong oxidizing agents.

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	(Vacated) TWA	400 ppm	1600 mg/m ³
	(Vacated) STEL	500 ppm	2000 mg/m ³
	TWA	500 ppm	2000 mg/m ³
Methylcyclohexane	(Vacated) TWA	400 ppm	1600 mg/m ³
	TWA	500 ppm	2000 mg/m ³

US. ACGIH Threshold Limit Values

Component	Type	Value
n-Heptane	TWA	400 ppm
	STEL	500 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/m3
	Ceiling	400 ppm	1800 mg/m3
Methylcyclohexane	IDLH	1200 ppm	
	TWA	400 ppm	1600 mg/m3

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.

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. Tight sealing safety goggles. Face protection shield.

Skin protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Body Protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory protection

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%
Lower	1.10%
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	log Pow: > 3
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	C7H16
Molecular Weight	100.20 g/mol
VOC Content(%)	No information available
Oxidizing properties	No information available

9.2 Other safety information

No information 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 (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) 4h
Methylcyclohexane	3200 mg/kg (Rat)	86700 mg/kg (Rabbit)	-

Skin corrosion/irritation

Irritating to eyes and skin.

Serious eye damage/eye irritation

No information available.

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

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.

11.2 Additional Information

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

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic organisms; may cause long-term adverse effects in the aquatic environment.

Product		Species	Test Results
n-Heptane	LC50	Freshwater Fish	375.0 mg/L, 96h
	EC50	Water Flea	>10 mg/L/24h
Methylcyclohexane	LC50	Freshwater Fish	2.07 mg/L, 96h, semi-static

12.2 Persistence and degradability

May persist.

12.3 Bio accumulative potential

No information available.

12.4 Mobility in soil

Not likely mobile in the environment due to its low water solubility.

12.5 Results of PBT and vPvB assessment

No information available.

12.6 Endocrine disrupting properties

No information available.

12.7 Other adverse effects

No information available.

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
Packing Group II

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 applicable.

CERCLA Hazardous Substance List (40 CFR 302.4)
Not applicable.

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 (CAS #142-82-5).

Listed, Methylcyclohexane (CAS #108-87-2).

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

Listed, n-Heptane (CAS #142-82-5).

Listed, Methylcyclohexane (CAS #108-87-2).

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

Listed, n-Heptane (CAS #142-82-5).

Listed, Methylcyclohexane (CAS #108-87-2).

Listed, Isooctane (CAS #26635-64-3).

California Proposition 65

Not listed.

SECTION 16: Other information

Issue date: 03/07/2017

Revision 1: 06/27/2023

Revision 2: 10/07/2024

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.