

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Hexane, mixture of isomers

Product Number : 227064

Brand : Sigma-Aldrich

Supplier : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

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Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555

Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards

Flammable liquid, Target Organ Effect, Harmful by ingestion., Irritant, Reproductive hazard

Target Organs

Peripheral nervous system., Kidney, Testes.

GHS Classification

Flammable liquids (Category 2)
Acute toxicity, Oral (Category 4)
Skin irritation (Category 2)
Eye irritation (Category 2A)
Reproductive toxicity (Category 2)
Specific target organ toxicity - single exposure (Category 3)
Specific target organ toxicity - repeated exposure, Oral (Category 2)
Specific target organ toxicity - repeated exposure, Inhalation (Category 2)
Aspiration hazard (Category 1)
Acute aquatic toxicity (Category 2)
Chronic aquatic toxicity (Category 2)

GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour.
H302 Harmful if swallowed.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 + H336 May cause respiratory irritation, and drowsiness or dizziness.

H361f Suspected of damaging fertility.
 H373 May cause damage to organs through prolonged or repeated exposure if swallowed.
 H373 May cause damage to organs through prolonged or repeated exposure if inhaled.
 H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
 P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
 P273 Avoid release to the environment.
 P281 Use personal protective equipment as required.
 P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
 P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P331 Do NOT induce vomiting.

HMIS Classification

Health hazard: 2
Chronic Health Hazard: *
Flammability: 3
Physical hazards: 0

NFPA Rating

Health hazard: 2
Fire: 3
Reactivity Hazard: 0

Potential Health Effects

Inhalation May be harmful if inhaled. Causes respiratory tract irritation. Vapours may cause drowsiness and dizziness.
Skin Harmful if absorbed through skin. Causes skin irritation.
Eyes Causes eye irritation.
Ingestion Harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Hexanes
 Isohexane

Formula : C₆H₁₄
 Molecular Weight : 86.18 g/mol

Component	Classification	Concentration
Methylcyclopentane		
CAS-No. 96-37-7 EC-No. 202-503-2	Flam. Liq. 2; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; Asp. Tox. 1; H225, H302, H304, H315, H319, H335	-
n-Hexane		
CAS-No. 110-54-3 EC-No. 203-777-6 Index-No. 601-037-00-0	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Chronic 2; H225, H304, H315, H336, H361f, H373, H411	50 - 70 %
Hexanes, isomers		
	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Chronic 2; H225, H304, H315, H336, H361f, H373, H411	10 - 30 %

2-Methylpentane			
CAS-No.	107-83-5	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Chronic 2; H225, H304, H315, H336, H411	1 - 5 %
EC-No.	203-523-4		
Index-No.	601-007-00-7		
3-Methylpentane			
CAS-No.	96-14-0	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Chronic 2; H225, H315, H304, H336, H411	1 - 5 %
EC-No.	202-481-4		
Index-No.	601-007-00-7		

For the full text of the H-Statements and R-Phrases mentioned in this Section, see Section 16

4. 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

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Conditions of flammability

Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.

Suitable extinguishing media

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

Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

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.

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.

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).

7. HANDLING AND STORAGE

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.

Conditions for safe storage

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.

Moisture sensitive. Handle and store under inert gas.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Components with workplace control parameters**

Components	CAS-No.	Value	Control parameters	Basis
n-Hexane	110-54-3	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
Remarks	Central Nervous System impairment Eye irritation Peripheral neuropathy Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Danger of cutaneous absorption			
		TWA	50 ppm 180 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	500 ppm 1,800 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
	The value in mg/m ³ is approximate.			
		TWA	50 ppm 180 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
2-Methylpentane	107-83-5	TWA	500 ppm 1,800 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	1,000 ppm 3,600 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	500 ppm 1,760 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		STEL	1,000 ppm 3,500 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		TWA	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
Remarks	Eye & Upper Respiratory Tract irritation Central Nervous System impairment			
		STEL	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Eye & Upper Respiratory Tract irritation Central Nervous System impairment			
		TWA	500 ppm 1,800 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	1,000 ppm 3,600 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	100 ppm 350 mg/m ³	USA. NIOSH Recommended Exposure Limits
	Also see specific listing for n-Hexane.			
		C	510 ppm 1,800 mg/m ³	USA. NIOSH Recommended Exposure Limits
	Also see specific listing for n-Hexane. 15 minute ceiling value			
3-Methylpentane	96-14-0	TWA	500 ppm 1,800 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000

		STEL	1,000 ppm 3,600 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	500 ppm 1,760 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		STEL	1,000 ppm 3,500 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		TWA	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
Remarks	Eye & Upper Respiratory Tract irritation Central Nervous System impairment			
		STEL	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Eye & Upper Respiratory Tract irritation Central Nervous System impairment			
		TWA	500 ppm 1,800 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	1,000 ppm 3,600 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	100 ppm 350 mg/m ³	USA. NIOSH Recommended Exposure Limits
	Also see specific listing for n-Hexane.			
		C	510 ppm 1,800 mg/m ³	USA. NIOSH Recommended Exposure Limits
	Also see specific listing for n-Hexane. 15 minute ceiling value			

Personal protective equipment

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).

Hand 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.

Eye 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 and 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.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	liquid
Colour	no data available

Safety data

pH	no data available
Melting	Melting point/range: -95 °C (-139 °F)

point/freezing point	
Boiling point	68 - 70 °C (154 - 158 °F) at 1,013 hPa (760 mmHg)
Flash point	no data available
Ignition temperature	no data available
Auto-ignition temperature	225 °C (437 °F)
Lower explosion limit	1.1 %(V)
Upper explosion limit	7.5 %(V)
Vapour pressure	no data available
Density	0.672 g/cm ³
Water solubility	no data available
Partition coefficient: n-octanol/water	no data available
Relative vapour density	no data available
Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

Vapours may form explosive mixture with air.

Conditions to avoid

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

Materials to avoid

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral LD50

no data available

Inhalation LC50

no data available

Dermal LD50

no data available

Other information on acute toxicity

no data available

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

Eyes: 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)

no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)

no data available

Aspiration hazard

no data available

Potential health effects

- | | |
|-------------------|---|
| Inhalation | May be harmful if inhaled. Causes respiratory tract irritation. Vapours may cause drowsiness and dizziness. |
| Ingestion | Harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage. |
| Skin | Harmful if absorbed through skin. Causes skin irritation. |
| Eyes | Causes eye irritation. |

Signs and Symptoms of Exposure

Prolonged or repeated contact with skin may cause:, defatting, Dermatitis, Contact with eyes can cause:, Redness, Blurred vision, Provokes tears., Effects due to ingestion may include:, Gastrointestinal discomfort, Central nervous system depression, Lung irritation, chest pain, pulmonary edema

Synergistic effects

no data available

Additional Information

RTECS: Not available

12. ECOLOGICAL INFORMATION**Toxicity**

no data available

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

Other adverse effects

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

13. DISPOSAL CONSIDERATIONS

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: 1208 Class: 3 Packing group: II
Proper shipping name: Hexanes
Reportable Quantity (RQ): 7692 lbs
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN number: 1208 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: HEXANES
Marine pollutant: No

IATA

UN number: 1208 Class: 3 Packing group: II
Proper shipping name: Hexanes

15. REGULATORY INFORMATION

OSHA Hazards

Flammable liquid, Target Organ Effect, Harmful by ingestion., Irritant, Reproductive hazard

SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
n-Hexane	110-54-3	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Methylcyclopentane	96-37-7	2007-03-01
n-Hexane	110-54-3	2007-07-01
2-Methylpentane	107-83-5	1993-04-24
3-Methylpentane	96-14-0	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Methylcyclopentane	96-37-7	2007-03-01

n-Hexane	110-54-3	2007-07-01
Hexanes, isomers	-	
2-Methylpentane	107-83-5	1993-04-24
3-Methylpentane	96-14-0	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Methylcyclopentane	96-37-7	2007-03-01
n-Hexane	110-54-3	2007-07-01
Hexanes, isomers	-	
2-Methylpentane	107-83-5	1993-04-24
3-Methylpentane	96-14-0	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

Text of H-code(s) and R-phras(e)s mentioned in Section 3

Acute Tox.	Acute toxicity
Aquatic Chronic	Chronic aquatic toxicity
Asp. Tox.	Aspiration hazard
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H361f	Suspected of damaging fertility.
H373	May cause damage to organs through prolonged or repeated exposure if inhaled.
H411	Toxic to aquatic life with long lasting effects.
Repr.	Reproductive toxicity
Skin Irrit.	Skin irritation
STOT RE	Specific target organ toxicity - repeated exposure
STOT SE	Specific target organ toxicity - single exposure

Further information

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