

**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Hexane, mixture of isomers  
Product Number : 227064  
Brand : Sigma-Aldrich

**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 : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA  
Telephone : +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  
Eye irritation (Category 2A), H319  
Reproductive toxicity (Category 2), H361  
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336  
Specific target organ toxicity - repeated exposure, Oral (Category 2), H373  
Specific target organ toxicity - repeated exposure, Inhalation (Category 2), H373  
Aspiration hazard (Category 1), H304  
Acute aquatic toxicity (Category 2), H401  
Chronic aquatic toxicity (Category 2), H411

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.  
H319 : Causes serious eye irritation.  
H336 : May cause drowsiness or dizziness.  
H361 : Suspected of damaging fertility or the unborn child.

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)	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
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.
P260	Do not breathe 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): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P331	Do NOT induce vomiting.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: 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 to extinguish.
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

#### 3.2 Mixtures

Synonyms	:	Hexanes Isohexane
Formula	:	C <sub>6</sub> H <sub>14</sub>
Molecular weight	:	86.18 g/mol

#### Hazardous components

Component	Classification	Concentration
<b>n-Hexane</b>		
CAS-No. EC-No. Index-No.	110-54-3 203-777-6 601-037-00-0	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H304, H315, H336, H361,

H373, H411			
<b>Hexanes, isomers</b>			
CAS-No.	92112-69-1	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H304, H315, H336, H361, H373, H411	>= 20 - < 30 %
<b>Methylcyclopentane</b>			
CAS-No.	96-37-7	Flam. Liq. 2; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; Asp. Tox. 1; H225, H302, H304, H315, H319, H335	>= 10 - < 20 %
EC-No.	202-503-2		
<b>2-Methylpentane</b>			
CAS-No.	107-83-5	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H304, H315, H336, H411	>= 1 - < 5 %
EC-No.	203-523-4		
Index-No.	601-007-00-7		
<b>3-Methylpentane</b>			
CAS-No.	96-14-0	Flam. Liq. 2; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H304, H315, H319, H336, H411	>= 1 - < 5 %
EC-No.	202-481-4		
Index-No.	601-007-00-7		

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

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.

### 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.

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## 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.

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## 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.

Moisture sensitive. Handle and store under inert gas.

Storage class (TRGS 510): Flammable liquids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
n-Hexane	110-54-3	TWA	50.000000 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	50.000000 ppm 180.000000 mg/m3	USA. NIOSH Recommended Exposure Limits	
		TWA	500.000000 ppm 1,800.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants	
		The value in mg/m3 is approximate.			
		TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)	
		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/m3	USA. NIOSH Recommended Exposure Limits	
		TWA	500 ppm 1,800 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants	
		The value in mg/m3 is approximate.			
		TWA	50 ppm 180 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000	
		PEL	50 ppm 180 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		Skin			
2-Methylpentane	107-83-5	TWA	500.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)	
		Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation			
		STEL	1,000.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)	
		Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation			
		TWA	100.000000 ppm 350.000000 mg/m3	USA. NIOSH Recommended Exposure Limits	
		Also see specific listing for n-Hexane.			
		C	510.000000 ppm 1,800.000000 mg/m3	USA. NIOSH Recommended Exposure Limits	
		Also see specific listing for n-Hexane. 15 minute ceiling value			

		STEL	1,000 ppm 3,600 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		PEL	500 ppm 1,800 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
3-Methylpentane	96-14-0	TWA	500.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)	
		Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation			
		STEL	1,000.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)	
		Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation			
		TWA	100.000000 ppm 350.000000 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits	
		Also see specific listing for n-Hexane.			
		C	510.000000 ppm 1,800.000000 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits	
		Also see specific listing for n-Hexane. 15 minute ceiling value			
		STEL	1,000 ppm 3,600 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	
		PEL	500 ppm 1,800 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)	

Hazardous components without workplace control parameters

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis	
n-Hexane	110-54-3	2,5-Hexanedione	0.4 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)	
	Remarks	End of shift at end of workweek				

## 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.

Full contact

Material: Nitrile rubber  
Minimum layer thickness: 0.4 mm  
Break through time: 480 min  
Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact  
Material: Nitrile rubber  
Minimum layer thickness: 0.2 mm  
Break through time: 30 min  
Material tested:Dermatril® P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### **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.

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## **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: -95 °C (-139 °F)
- f) Initial boiling point and boiling range 68 - 70 °C (154 - 158 °F) at 1,013 hPa (760 mmHg)
- g) Flash point No data available
- h) Evaporation rate No data available
- i) Flammability (solid, gas) No data available
- j) Upper/lower flammability or explosive limits Upper explosion limit: 7.5 %(V)  
Lower explosion limit: 1.1 %(V)
- k) Vapour pressure No data available
- l) Vapour density No data available
- m) Relative density 0.672 g/cm<sup>3</sup>
- n) Water solubility No data available
- o) Partition coefficient: n-octanol/water No data available

- p) Auto-ignition temperature 225 °C (437 °F)
- 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

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## 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.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### 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.

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  
No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

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

Testes. - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence (Hexanes, isomers)

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## 12. ECOLOGICAL INFORMATION

**12.1 Toxicity**

No data available

**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.  
Toxic to aquatic life with long lasting effects.

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## 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.

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## 14. TRANSPORT INFORMATION

**DOT (US)**

UN number: 1208      Class: 3

Packing group: II

Proper shipping name: Hexanes

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

**IMDG**

UN number: 1208      Class: 3  
Proper shipping name: HEXANES  
Marine pollutant:yes  
**IATA**  
UN number: 1208      Class: 3  
Proper shipping name: Hexanes

Packing group: II

EMS-No: F-E, S-D

Packing group: II

## 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

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

### Massachusetts Right To Know Components

	CAS-No.	Revision Date
n-Hexane	110-54-3	2007-07-01
Methylcyclopentane	96-37-7	1993-04-24
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
n-Hexane	110-54-3	2007-07-01
Hexanes, isomers	92112-69-1	
Methylcyclopentane	96-37-7	1993-04-24
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
n-Hexane	110-54-3	2007-07-01
Hexanes, isomers	92112-69-1	
Methylcyclopentane	96-37-7	1993-04-24
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

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

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic 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.
H361	Suspected of damaging fertility or the unborn child.

H373	May cause damage to organs (/*_ORG REP ORAL/) through prolonged or repeated exposure if swallowed.
H401	Toxic to aquatic life.
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

#### **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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#### **Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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