

SAFETY DATA SHEET

Version 6.9
Revision Date 11/27/2023
Print Date 05/11/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Hexane, mixture of isomers

Product Number : 156175

Brand : SIGALD

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 Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

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), H225

Skin irritation (Category 2), H315

Reproductive toxicity (Category 2), H361

Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

Specific target organ toxicity - repeated exposure, Inhalation (Category 2), H373

Aspiration hazard (Category 1), H304

Short-term (acute) aquatic hazard (Category 2), H401

Long-term (chronic) aquatic hazard (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

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Pictogram



Signal Word

Danger

Hazard Statements

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin 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 inhaled.
H411	Toxic to aquatic life with long lasting effects.

Precautionary Statements

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/ vapors/ 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.
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.
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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : Hexanes
Isohexane

Molecular weight : 86.18 g/mol

Component		Classification	Concentration
n-Hexane			
CAS-No.	110-54-3	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H361, H336, H373, H304, H401, H411 Concentration limits: >= 5 %: STOT RE 2, H373; >= 20 %: STOT SE 3, H336;	>= 50 - < 70 %
EC-No.	203-777-6		
Index-No.	601-037-00-0		
Registration number	01-2119480412-44-XXXX		
Hexanes, isomers			
CAS-No.	92112-69-1	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; Asp. Tox. 1; Aquatic Chronic 2; H225, H315, H361, H336, H304, H411	>= 20 - < 30 %
EC-No.	295-570-2		
Index-No.	601-037-00-0		
methylcyclopentane			
CAS-No.	96-37-7	Flam. Liq. 2; Asp. Tox. 1; H225, H304	>= 10 - < 20 %
EC-No.	202-503-2		
2-Methylpentane			
CAS-No.	107-83-5	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H336, H304, H401, 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; Eye Irrit. 2A; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H315, H319, H336, H304, H401, 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.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

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 let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). 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

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive 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

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Moisture sensitive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
n-Hexane	110-54-3	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	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
		PEL	50 ppm 180 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Hexanes, isomers	92112-69-1	TWA	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		STEL	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		TWA	100 ppm 350 mg/m3	USA. NIOSH Recommended Exposure Limits
		C	510 ppm 1,800 mg/m3	USA. NIOSH Recommended Exposure Limits
		PEL	500 ppm 1,800 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	1,000 ppm 3,600 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
2-Methylpentane	107-83-5	TWA	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		STEL	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		TWA	100 ppm 350 mg/m3	USA. NIOSH Recommended Exposure Limits
		C	510 ppm 1,800 mg/m3	USA. NIOSH Recommended Exposure Limits
		PEL	500 ppm 1,800 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	1,000 ppm 3,600 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
3-methylpentane	96-14-0	TWA	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		STEL	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		TWA	100 ppm 350 mg/m3	USA. NIOSH Recommended Exposure Limits
		C	510 ppm 1,800 mg/m3	USA. NIOSH Recommended Exposure Limits
		PEL	500 ppm 1,800 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	1,000 ppm 3,600 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
n-Hexane	110-54-3	2,5-Hexanedione	0.5 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift			

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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.

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

- | | |
|--|---------------------------------------|
| a) Appearance | Form: liquid |
| b) Odor | No data available |
| c) Odor 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 |

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) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	0.672 g/cm ³
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	225 °C (437 °F)
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	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

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Inhalation: No data available

Acute toxicity estimate Dermal - 3,846 mg/kg
(Calculation method)

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient 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 ingredient 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 on OSHA's list of regulated carcinogens.

Reproductive toxicity

Suspected of damaging the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Mixture may cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

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

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Components

n-Hexane

Acute toxicity

LD50 Oral - Rat - male and female - 16,000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - 172 mg/l - vapor

Remarks: (RTECS)

LD50 Dermal - Rabbit - male - > 2,000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 24 h

(OECD Test Guideline 404)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h

(OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 478

Species: Mouse - male

Result: negative

Method: OECD Test Guideline 475

Species: Rat - male and female - Bone marrow

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

Inhalation - May cause damage to organs through prolonged or repeated exposure.
- Nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

Hexanes, isomers

Acute toxicity

Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation

Remarks: Causes skin irritation.
Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: 2-Methylpentane

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: 2-Methylpentane

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways.

methylcyclopentane

Acute toxicity

Oral: No data available
Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

2-Methylpentane

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways.

3-methylpentane**Acute toxicity**

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways.

SECTION 12: Ecological information**12.1 Toxicity****Mixture**

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

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12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

n-Hexane

Toxicity to fish

LC50 - Pimephales promelas (fathead minnow) - 2.5 mg/l - 96 h
Remarks: (ECOTOX Database)

Toxicity to daphnia
and other aquatic
invertebrates

EC50 - Daphnia magna (Water flea) - 2.1 mg/l - 48 h
Remarks: (Lit.)

Hexanes, isomers

No data available

methylcyclopentane

No data available

2-Methylpentane

No data available

3-methylpentane

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1208 Class: 3

Packing group: II

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Proper shipping name: Hexanes
Reportable Quantity (RQ):
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 : yes
Marine pollutant : yes

IATA

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

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

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	2020-07-14

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
n-Hexane	110-54-3	2020-07-14
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

n-Hexane	CAS-No. 110-54-3	Revision Date 2020-07-14
methylcyclopentane	96-37-7	1993-04-24
2-Methylpentane	107-83-5	1993-04-24

California Prop. 65 Components

, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov. n-Hexane

CAS-No.
110-54-3

Revision Date
2017-12-29

SECTION 16: Other information**Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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