SAFETY DATA SHEET

Version 6.11
Revision Date 12/18/2024
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Heptane

Product Number : 650536
Brand : SIGALD
Index-No. : 601-008-00-2
CAS-No. : 142-82-5

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

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

GHS label elements

Hazard pictograms :

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.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary Statements :

Prevention:

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.
P261 Avoid breathing mist or vapors.
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/ eye protection/ face protection.

Response:

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.
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.

Storage:

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.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS-No.	Concentration (% w/w)
n-heptane	142-82-5	>= 90 - <= 100

Actual concentration is withheld as a trade secret

SECTION 4. 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.

In case of eye contact : After eye contact: rinse out with plenty of water. 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.

Most important symp- : The most important known symptoms and effects are

toms and effects, both acute and delayed		described in the labelling (see section 2.2) and/or in section 11
Protection of first-aiders	:	For personal protection see section 8.
Notes to physician	:	No data available

SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media	:	Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Flash back possible over considerable distance. 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.
Hazardous combustion products	:	Carbon oxides
Specific extinguishing methods	:	No data available
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.
Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

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. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter drains. Risk of explosion.
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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	:	Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	:	Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Conditions for safe storage	:	Store under inert gas.
Further information on storage conditions	:	Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class	:	3, Flammable liquids
Recommended storage temperature	:	Recommended storage temperature see product label.
Packaging material	:	Suitable material: Mild Steel Drum, Amber Glass Bottle/Jar

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
n-heptane	142-82-5	TWA	85 ppm 350 mg/m3	NIOSH REL
		C	440 ppm 1,800 mg/m3	NIOSH REL
		TWA	500 ppm 2,000 mg/m3	OSHA Z-1
		TWA	400 ppm	ACGIH
		STEL	500 ppm	ACGIH

Engineering measures : No data available

Personal protective equipment

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.

Recommended Filter type: : Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepeneur 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.

Filter type ABEK

Hand protection

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0.4 mm
Protective index	:	Full contact
Manufacturer	:	Camatril® (KCL 730 / Aldrich Z677442, Size M)
Material	:	Nitrile rubber
Break through time	:	60 min
Glove thickness	:	0.2 mm
Protective index	:	Splash contact
Manufacturer	:	Dermatril® P (KCL 743 / Aldrich Z677388, Size M)
Remarks	:	This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	:	Flame retardant antistatic protective clothing.
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	liquid
Color	:	No data available
Odor	:	No data available
Odor Threshold	:	No data available
pH	:	No data available
Melting point	:	-131.8 °F / -91.0 °C

Boiling point/boiling range	:	208.8 - 209.1 °F / 98.2 - 98.4 °C (1,000 hPa)
Flash point	:	25 °F / -4 °C Method: c.c., closed cup
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Self-ignition	:	433.4 °F / 223.0 °C
Upper explosion limit / Upper flammability limit	:	Upper explosion limit 7 %(V)
Lower explosion limit / Lower flammability limit	:	1.1 %(V)
Vapor pressure	:	48 hPa (68.0 °F / 20.0 °C)
Relative vapor density	:	No data available
Relative density	:	No data available
Density	:	0.68 g/cm3 (59 °F / 15 °C)
Solubility(ies) Water solubility	:	insoluble
Partition coefficient: n-octanol/water	:	log Pow: > 3 Bioaccumulation is not expected.
Autoignition temperature	:	433 °F / 223 °C
Decomposition temperature	:	No data available
Viscosity Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	0.64 mm2/s (68 °F / 20 °C)
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none

Molecular weight	:	100.20 g/mol
Particle characteristics		
Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	Vapors may form explosive mixture with air.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	Risk of ignition or formation of inflammable gases or vapours with: Strong oxidizing agents phosphorus in the presence of: Chlorine
Conditions to avoid	:	Warming.
Incompatible materials	:	rubber various plastics
Hazardous decomposition products	:	In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - > 5,000 mg/kg
(OECD Test Guideline 401)
Remarks: The value is given in analogy to the following substances: isooctane
LC50 Inhalation - Rat - male and female - 4 h - > 29.29 mg/l - vapor

(OECD Test Guideline 403)
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)
Remarks: The value is given in analogy to the following substances: isooctane

Skin corrosion/irritation
Skin - Rabbit
Result: Irritating to skin. - 24 h
(OECD Test Guideline 404)
Remarks: The value is given in analogy to the following substances: isooctane
Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)
Remarks: The value is given in analogy to the following substances: isooctane

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: negative
(OECD Test Guideline 406)
Remarks: **Germ cell mutagenicity**
Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: rat hepatocytes
Method: OECD Test Guideline 473
Result: negative

Carcinogenicity
This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

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
No data available

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)

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
May be fatal if swallowed and enters airways.
Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

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.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

n-heptane:

Toxicity to fish	:	LL50 (Rainbow darter (Etheostoma caeruleum)): > 13.4 mg/l Exposure time: 96 h Method: OECD Test Guideline 203 Remarks: (ECHA)
Toxicity to daphnia and other aquatic inverte-brates	:	EC50 (Daphnia magna (Water flea)): 0.23 mg/l Exposure time: 21 d Test Type: static test Analytical monitoring: yes GLP: yes Remarks: (ECHA) (in analogy to similar products)
Toxicity to algae/aquatic plants	:	EL50 (Pseudokirchneriella subcapitata (green algae)): 29 mg/l End point: Growth inhibition Exposure time: 72 h Method: OECD Test Guideline 201 GLP: yes Remarks: (ECHA) NOELR (Pseudokirchneriella subcapitata (green algae)): 6.3 mg/l End point: Growth inhibition Exposure time: 72 h Method: OECD Test Guideline 201 GLP: yes Remarks: (ECHA)
M-Factor (Acute aquatic toxicity)	:	1
M-Factor (Chronic aquatic toxicity)	:	1

Ecotoxicology Assessment

Acute aquatic toxicity	:	Very toxic to aquatic life.

Chronic aquatic toxicity	:	Very toxic to aquatic life with long lasting effects.

Persistence and degradability

Components:

n-heptane:

Biodegradability	:	aerobic Concentration: 3.3 mg/l Result: Readily biodegradable. Biodegradation: 70 % Exposure time: 10 d Remarks: (ECHA)
Biochemical Oxygen Demand (BOD)	:	1,920 mg/g Incubation time: 5 d Remarks: (IUCLID)
ThOD	:	3,500 mg/g Remarks: (Lit.)
BOD/ThOD	:	55 % Remarks: (Lit.)

Bioaccumulative potential

Components:

n-heptane:

Bioaccumulation	:	Remarks: Indication of bioaccumulation.
Partition coefficient: n-octanol/water	:	log Pow: > 3 Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential	:	Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

n-heptane:

Results of PBT and vPvB	:	Substance does not meet the criteria for PBT or vPvB

assessment		according to Regulation (EC) No 1907/2006, Annex XIII.
Additional ecological information	:	Do not empty into drains. Avoid release to the environment.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues	:	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

International Regulations

IATA-DGR

UN/ID No.	:	UN 1206
Proper shipping name	:	Heptanes
Class	:	3
Packing group	:	II
Labels	:	Class 3 - Flammable liquids
Packing instruction (cargo aircraft)	:	364
Packing instruction (passenger aircraft)	:	353

IMDG-Code

UN number	:	UN 1206
Proper shipping name	:	HEPTANES
Class	:	3
Packing group	:	II
Labels	:	3
EmS Code	:	F-E, S-D
Marine pollutant	:	yes

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation

49 CFR Road

UN/ID/NA number	:	UN 1206
Proper shipping name	:	Heptanes
Class	:	3
Packing group	:	II
Labels	:	Class 3 - Flammable liquids

ERG Code	:	128
Marine pollutant	:	yes
Poison Inhalation Hazard	:	No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312 Hazards	:	Fire Hazard Acute Health Hazard Chronic Health Hazard
SARA 313	:	This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).
This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.
This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.
This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307
This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

n-heptane	142-82-5

Pennsylvania Right To Know

n-heptane	142-82-5

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	:	USA. NIOSH Recommended Exposure Limits
OSHA Z-1	:	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	:	8-hour, time-weighted average
ACGIH / STEL	:	Short-term exposure limit
NIOSH REL / TWA	:	Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
NIOSH REL / C	:	Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA	:	8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - Inter-

national Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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.

Revision Date : 12/18/2024

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