

SAFETY DATA SHEET

Version 6.5
Revision Date 01.03.2024
Print Date 30.07.2024

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

1.1 Product identifiers

Product name : Heptane

Product Number : 650536
Brand : SIGALD
CAS-No. : 142-82-5

1.2 Other means of identification

No data available

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

Identified uses : For R&D use only. Not for pharmaceutical, household or other uses.

1.4 Details of the supplier of the safety data sheet

Company : Merck Life Science Pty Ltd
Ground Floor, Building 1, 885 Mountain Highway
BAYSWATER VIC 3153
AUSTRALIA

Telephone : +61 1800 800 097
E-mail address : customersupport.anz@merckgroup.com

1.5 Emergency telephone

Emergency Phone # : Free call (24/7): 1800 862 115
Int'l (24/7): +61 2 9037 2994
(CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

Flammable liquids (Category 2), H225
Skin corrosion/irritation (Category 2), H315
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

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 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, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233

Keep container tightly closed.

P261

Avoid breathing mist or vapors.

P264

Wash skin thoroughly after handling.

P273

Avoid release to the environment.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P310

IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

P331

Do NOT induce vomiting.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391

Collect spillage.

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

Formula

: C₇H₁₆

Molecular weight

: 100.20 g/mol

CAS-No.

: 142-82-5

EC-No.

: 205-563-8

Index-No.

: 601-008-00-2

Hazardous ingredients

Component	Classification	Concentration
n-heptane		
	Flam. Liq. 2; Skin Corr./Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304,	<= 100 %

	H400, H410 Concentration limits: 20 %: STOT SE 3, H336; M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	
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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.

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.

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

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.

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

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.

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

Store under inert gas.

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

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.3 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-heptane	142-82-5	STEL	500 ppm 2,050 mg/m ³	Australia. Workplace Exposure Standards for Airborne Contaminants.
		TWA	400 ppm 1,640 mg/m ³	Australia. Workplace Exposure Standards for Airborne Contaminants.

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

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).

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)

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).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm

Break through time: 60 min

Material tested: Dermatril® P (KCL 743 / Aldrich Z677388, Size M)

Body Protection

Flame retardant antistatic protective clothing.

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.

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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) Physical state	liquid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	Melting point: -91.0 °C
e) Initial boiling point and boiling range	98.2 - 98.4 °C at 1,000 hPa
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 7 %(V) Lower explosion limit: 1.1 %(V)
h) Flash point	-4 °C - c.c.
i) Autoignition temperature	223.0 °C
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: 0.64 mm ² /s at 20 °C Viscosity, dynamic: No data available
m) Water solubility	insoluble
n) Partition coefficient: n-octanol/water	log Pow: > 3 - Bioaccumulation is not expected.
o) Vapor pressure	48 hPa at 20.0 °C
p) Density	0.68 g/cm ³ at 15 °C

Relative density	No data available
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
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

Risk of ignition or formation of inflammable gases or vapours with:

Strong oxidizing agents

phosphorus

in the presence of:

Chlorine

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, various plastics

10.6 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.

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.

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 10 d
Result: 70 % - Readily biodegradable.
Remarks: (ECHA)

Biochemical Oxygen 1,920 mg/g
Demand (BOD) Remarks: (IUCLID)

Theoretical oxygen 3,500 mg/g
demand Remarks: (Lit.)

Ratio BOD/ThBOD 55 %
Remarks: (Lit.)

12.3 Bioaccumulative potential

Indication of bioaccumulation.

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Additional ecological Do not empty into drains. Avoid release to the environment.
information

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

14.1 UN number

ADR/RID: 1206

IMDG: 1206

IATA-DGR: 1206

14.2 UN proper shipping name

ADR/RID: HEPTANES

IMDG: HEPTANES

IATA-DGR: Heptanes

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA-DGR: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA-DGR: no

14.6 Special precautions for user

None

14.7 Incompatible materials

rubber, various plastics

Other regulations

Hazchem Code : 3YE

SECTION 15: Regulatory information**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**Therapeutic Goods (Poisons Standard)
Instrument: No poison schedule number
allocated

SECTION 16: Other information

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

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.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

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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