

SAFETY DATA SHEET

Version 6.5
Revision Date 04.03.2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Octane

Product Number : 412236
Brand : SIGALD
Index-No. : 601-009-00-8
CAS-No. : 111-65-9

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 : MilliporeSigma Canada Ltd.
2149 WINSTON PARK DRIVE
OAKVILLE ON L6H 6J8
CANADA

Telephone : +1 905 829-9500
Fax : +1 905 829-9292

1.4 Emergency telephone

Emergency Phone # : +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 Hazardous Products Regulations (HPR) (SOR/2015-17)**

Flammable liquids (Category 2), H225
Skin 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

| | |
|--------------------|---|
| P210 | Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. |
| P233 | Keep container tightly closed. |
| P240 | Ground and bond container and receiving equipment. |
| P241 | Use explosion-proof electrical/ ventilating/ lighting/ equipment. |
| P242 | Use non-sparking tools. |
| P243 | Take action to prevent static discharges. |
| 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/ 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. |
| 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 + P364 | Take off contaminated clothing and wash it 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

3.1 Substances

Synonyms : n-Octane
SIGALD - 412236

Page 2 of 12

Formula : C₈H₁₈
 Molecular weight : 114.23 g/mol
 CAS-No. : 111-65-9
 EC-No. : 203-892-1
 Index-No. : 601-009-00-8

| Component | Classification | Concentration * |
|-----------------|---|--------------------|
| n-octane | | |
| | Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 | <= 100 % |
| * Weight % | | |

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

Carbon dioxide (CO₂) Foam 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.

hygroscopic

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

| Components | CAS-No. | Value | Control parameters | Basis |
|------------|--|-------|------------------------------------|---|
| n-octane | 111-65-9 | TWA | 300 ppm 1,400 mg/m ³ | Canada. Alberta, Occupational Health and Safety Code (table 2: OEL) |
| Remarks | Occupational exposure limit is based on irritation effects and its adjustment to compensate for unusual work schedules is not required | | | |
| | | TWAEV | 300 ppm | Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants |
| | | TWA | 300 ppm | Canada. British Columbia OEL |
| | | TWA | 300 ppm | USA. ACGIH Threshold Limit Values (TLV) |

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: 0.11 mm

Break through time: 30 min

Material tested: KCL 741 Dermatril® L

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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

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 Color: colorless |
| b) Odor | characteristic |

| | |
|---|---|
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: -57 °C (-71 °F) - lit. |
| f) Initial boiling point and boiling range | 125 - 127 °C 257 - 261 °F - lit. |
| g) Flash point | 13 °C (55 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 6.5 %(V) Lower explosion limit: 0.96 %(V) |
| k) Vapor pressure | 14.7 hPa at 20.0 °C (68.0 °F) |
| l) Vapor density | No data available |
| m) Density | 0.703 g/cm ³ at 25 °C (77 °F) - lit. |
| Relative density | No data available |
| n) Water solubility | ca.0.007 g/l at 20 °C (68 °F) |
| o) Partition coefficient: n-octanol/water | log Pow: 5.15 |
| p) Autoignition temperature | 220 °C (428 °F) |
| q) Decomposition temperature | No data available |
| r) Viscosity | 0.8 mm ² /s at 20 °C (68 °F) - |
| 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

Violent reactions possible with:
Strong oxidizing agents

SIGALD - 412236

Page 7 of 12

various plastics

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

No data available

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 - > 24.88 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: (in analogy to similar products)

The value is given in analogy to the following substances: isooctane

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

Remarks: Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation
(OECD Test Guideline 405)

Remarks: (in analogy to similar products)

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: (in analogy to similar products)

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

Remarks: The value is given in analogy to the following substances: n-heptane
Test Type: Chromosome aberration test in vitro

Test system: rat hepatocytes

Method: OECD Test Guideline 473

Result: negative

Remarks: The value is given in analogy to the following substances: n-heptane
Test Type: In vitro mammalian cell gene mutation test

Test system: human lymphoblastoid cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances:

isooctane
Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - 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

No data available

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

RTECS: RG8400000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Vomiting, Central nervous system depression, narcosis

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

Systemic effects:

After uptake of large quantities:

Headache

Dizziness

Nausea

Vomiting

agitation

somnolence

Drowsiness

Unconsciousness

respiratory arrest

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

| | |
|---|--|
| Toxicity to fish | LC50 - <i>Oryzias latipes</i> - 0.42 mg/l - 96.0 h Remarks: (Lit.) |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - <i>Daphnia magna</i> (Water flea) - 0.38 mg/l - 48 h Remarks: (ECOTOX Database) |
| Toxicity to algae | NOEC - <i>Pseudokirchneriella subcapitata</i> (microalgae) - 5.8 mg/l - 72 h Remarks: (Lit.) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | static test NOEC - <i>Daphnia magna</i> (Water flea) - 0.17 mg/l - 21 d (OECD Test Guideline 211) Remarks: (in analogy to similar products) |

12.2 Persistence and degradability

| | |
|------------------|--|
| Biodegradability | aerobic - Exposure time 10 d Result: 70.3 % - Readily biodegradable. Remarks: (ECHA) |
|------------------|--|

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

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

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.

SECTION 14: Transport information

TDG

UN number: 1262 Class: 3 Packing group: II
Proper shipping name: OCTANES
Labels: 3
ERG Code: 128
Marine pollutant: no

IMDG

UN number: 1262 Class: 3 Packing group: II EMS-No: F-E, S-E
Proper shipping name: OCTANES
Marine pollutant : yes
Marine pollutant : yes

IATA

UN number: 1262 Class: 3 Packing group: II
Proper shipping name: Octanes

SECTION 15: Regulatory information

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

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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