

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Octane

Product Number : 412236
Brand : Sigma-Aldrich
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, Manufacture 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 # : (314) 776-6555

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
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
Aspiration hazard (Category 1), H304
Acute aquatic toxicity (Category 1), H400
Chronic aquatic toxicity (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 statement(s)

H225 Highly flammable liquid and vapour.
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 statement(s)

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 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 or doctor/ physician. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P304 + P340 | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. |
| P312 | Call a POISON CENTER or doctor/ physician if you feel unwell. |
| P321 | Specific treatment (see supplemental first aid instructions on this label). |
| 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 for extinction. |
| 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

3.1 Substances

| | |
|------------------|----------------------------------|
| Synonyms | : n-Octane |
| Formula | : C ₈ H ₁₈ |
| Molecular Weight | : 114.23 g/mol |
| CAS-No. | : 111-65-9 |
| EC-No. | : 203-892-1 |
| Index-No. | : 601-009-00-8 |

Hazardous components

| Component | Classification | Concentration |
|---------------|---|---------------|
| Octane | | |
| | Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H304, H315, H336, H410 | - |

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

Flush eyes with water as a precaution.

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**

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

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.

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

Store in cool place. 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.

hygroscopic

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

| Component | CAS-No. | Value | Control parameters | Basis |
|-----------|----------|--|------------------------------------|--|
| Octane | 111-65-9 | TWA | 300 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Upper Respiratory Tract irritation | | |
| | | TWA | 75 ppm 350 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | C | 385 ppm 1,800 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | 15 minute ceiling value | | |
| | | TWA | 500 ppm 2,350 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | The value in mg/m ³ is approximate. | | |
| | | TWA | 300 ppm 1,450 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | STEL | 375 ppm 1,800 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |

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: 0.2 mm

Break through time: 480 min

Material tested: Dermatrill® 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

| | |
|---|---|
| a) Appearance | Form: liquid Colour: colourless |
| b) Odour | characteristic |
| c) Odour 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 | 13.0 °C (55.4 °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) Vapour pressure | 14.7 hPa (11.0 mmHg) at 20.0 °C (68.0 °F) |
| l) Vapour density | no data available |
| m) Relative density | 0.703 g/cm ³ at 25 °C (77 °F) |
| n) Water solubility | ca.0.007 g/l at 20 °C (68 °F) |
| o) Partition coefficient: n-octanol/water | log Pow: 5.15 |
| p) Auto-ignition temperature | 220.0 °C (428.0 °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

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. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

Strong acids, Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LC50 Inhalation - rat - 4 h - 118,000 mg/m³

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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

Additional Information

RTECS: RG8400000

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish mortality LC50 - *Oryzias latipes* - 0.42 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates Immobilization EC50 - *Daphnia magna* (Water flea) - 0.38 mg/l - 48 h

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.**

| | |
|-----------------|---|
| Aquatic Acute | Acute aquatic toxicity |
| Aquatic Chronic | Chronic aquatic toxicity |
| Asp. Tox. | Aspiration hazard |
| Flam. Liq. | Flammable liquids |
| H225 | Highly flammable liquid and vapour. |
| 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. |
| Skin Irrit. | Skin irritation |

HMIS Rating

| | |
|------------------------|---|
| Health hazard: | 0 |
| 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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