

## SAFETY DATA SHEET

Version 5.6  
Revision Date 08/14/2018  
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**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, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Canada Co.  
2149 Winston Park Drive  
OAKVILLE ON L6H 6J8  
CANADA  
  
Telephone : +1 9058299500  
Fax : +1 9058299292

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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**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  
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, 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 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/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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |                                  |
|------------------|----------------------------------|
| Synonyms         | : n-Octane                       |
| Formula          | : C <sub>8</sub> H <sub>18</sub> |
| 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* |
|------------------|---|----------------|
| <b>n-octane</b>  |   |                |
|                  | Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H304, H315, H336, H410 | 90 - 100 %     |
| * Weight percent |   |                |

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

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**5. FIREFIGHTING MEASURES****5.1 Extinguishing media****Suitable extinguishing media**

Dry powder Dry sand

**Unsuitable extinguishing media**

Do NOT use water jet.

**5.2 Special hazards arising from the substance or mixture**

No data available

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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**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 non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

**6.4 Reference to other sections**

For disposal see section 13.

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**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**

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

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

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

Components with workplace control parameters

| Components | CAS-No.  | Value | Control parameters                 | Basis   |
|------------|--|-------|------------------------------------|---|
| n-octane   | 111-65-9   | TWA   | 300 ppm<br>1,400 mg/m <sup>3</sup> | 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<br>1,400 mg/m <sup>3</sup> | Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants |
|            |  | STEV  | 375 ppm<br>1,750 mg/m <sup>3</sup> | 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

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: Dermatril® 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |   |
|---|---|
| a) Appearance                                   | Form: liquid<br>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 °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)<br>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 <sup>3</sup> 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 °C (428 °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

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## 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.

#### 10.5 Incompatible materials

Strong acids, Strong oxidizing agents

#### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

##### Acute toxicity

LC50 Inhalation - Rat - 4 h - 118,000 mg/m<sup>3</sup>

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.

##### 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

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### 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

Toxicity to algae                      Growth inhibition NOEC - Pseudokirchneriella subcapitata (microalgae) - 5.8 mg/l - 72 h

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

12.6 Other adverse effects  
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Very toxic to aquatic life with long lasting effects.

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### 13. DISPOSAL CONSIDERATIONS

#### 13.1 Waste treatment methods

##### Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

##### Contaminated packaging

Dispose of as unused product.

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### 14. TRANSPORT INFORMATION

#### TDG (Canada)

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

#### 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

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### 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.

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### 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

Further information

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