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/ eye protection/ face protection.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
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 or doctor/ physician 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.
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 : C₈H₁₈
Molecular weight : 114.23 g/mol
CAS-No. : 111-65-9
EC-No. : 203-892-1
Index-No. : 601-009-00-8

Hazardous components

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octane</td>
<td>Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H304, H315, H336, H410</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

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.

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
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): 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/PERSOAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octane</td>
<td>111-65-9</td>
<td>TWA</td>
<td>300.000000 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

Remarks: Upper Respiratory Tract irritation

<table>
<thead>
<tr>
<th>TWA</th>
<th>75.000000 ppm</th>
<th>350.000000 mg/m3</th>
<th>USA. NIOSH Recommended Exposure Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>385.000000 ppm</td>
<td>1,800.000000 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
</tbody>
</table>

15 minute ceiling value

<table>
<thead>
<tr>
<th>TWA</th>
<th>500.000000 ppm</th>
<th>2,350.000000 mg/m3</th>
<th>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</th>
</tr>
</thead>
</table>

The value in mg/m3 is approximate.

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</tr>
</thead>
</table>

Upper Respiratory Tract irritation

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.

### 9. PHYSICAL AND CHEMICAL PROPERTIES

**9.1 Information on basic physical and chemical properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: liquid</td>
</tr>
<tr>
<td></td>
<td>Colour: colourless</td>
</tr>
<tr>
<td>b) Odour</td>
<td>characteristic</td>
</tr>
<tr>
<td>c) Odour Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>Melting point/range: -57 °C (-71 °F) - lit.</td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>125 - 127 °C (257 - 261 °F) - lit.</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>13 °C (55 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>Upper explosion limit: 6.5 %(V) Lower explosion limit: 0.96 %(V)</td>
</tr>
<tr>
<td>k) Vapour pressure</td>
<td>14.7 hPa (11.0 mmHg) at 20.0 °C (68.0 °F)</td>
</tr>
<tr>
<td>l) Vapour density</td>
<td>No data available</td>
</tr>
<tr>
<td>m) Relative density</td>
<td>0.703 g/cm3 at 25 °C (77 °F)</td>
</tr>
<tr>
<td>n) Water solubility</td>
<td>ca.0.007 g/l at 20 °C (68 °F)</td>
</tr>
<tr>
<td>o) Partition coefficient: n-octanol/water</td>
<td>log Pow: 5.15</td>
</tr>
<tr>
<td>p) Auto-ignition temperature</td>
<td>220 °C (428 °F)</td>
</tr>
<tr>
<td>q) Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>r) Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>s) Explosive properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>
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.

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
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.

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.

14. TRANSPORT INFORMATION
DOT (US)
UN number: 1262    Class: 3
Proper shipping name: Octanes
Reportable Quantity (RQ):
Poison Inhalation Hazard: No
Packing group: II

IMDG
UN number: 1262    Class: 3
Proper shipping name: OCTANES
Marine pollutant:yes
EM-S-No: F-E, S-E
Packing group: II
IATA
15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
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.

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octane</td>
<td>111-65-9</td>
<td>1993-04-24</td>
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</table>

Pennsylvania Right To Know Components

<table>
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<th>Component</th>
<th>CAS-No.</th>
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New Jersey Right To Know Components

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<tr>
<td>Octane</td>
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<td>1993-04-24</td>
</tr>
</tbody>
</table>

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: 2
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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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

**Preparation Information**
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.5 Revision Date: 06/30/2015 Print Date: 10/29/2015