1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Octane
Product Number : 412236
Brand : Sigma-Aldrich
Supplier : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO  63103
USA
Telephone : +1 800-325-5832
Fax : +1 800-325-5052
Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555
Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards
Flammable liquid, Irritant

Target Organs
Central nervous system

GHS Classification
Flammable liquids (Category 2)
Skin irritation (Category 2)
Specific target organ toxicity - single exposure (Category 3)
Aspiration hazard (Category 1)
Acute aquatic toxicity (Category 1)
Chronic aquatic toxicity (Category 4)

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.
H400 Very toxic to aquatic life.
H413 May cause long lasting harmful effects to aquatic life.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P273 Avoid release to the environment.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician.
P331  Do NOT induce vomiting.

HMIS Classification
- Health hazard: 0
- Flammability: 3
- Physical hazards: 0

NFPA Rating
- Health hazard: 2
- Fire: 3
- Reactivity Hazard: 0

Potential Health Effects

Inhalation  May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.

Skin  May be harmful if absorbed through skin. May cause skin irritation.

Eyes  May cause eye irritation.

Ingestion  May be harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms: n-Octane

Formula: C₈H₁₈
Molecular Weight: 114.23 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octane</td>
<td></td>
</tr>
<tr>
<td>CAS-No.</td>
<td>111-65-9</td>
</tr>
<tr>
<td>EC-No.</td>
<td>203-892-1</td>
</tr>
<tr>
<td>Index-No.</td>
<td>601-009-00-8</td>
</tr>
</tbody>
</table>

4. 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.

5. FIREFIGHTING MEASURES

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.

Special protective equipment for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.
Hazardous combustion products
Hazardous decomposition products formed under fire conditions. - Carbon oxides

Further information
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions
Use personal protective equipment. Avoid breathing vapors, 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.

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.

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).

7. HANDLING AND STORAGE

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.

Conditions for safe storage
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.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

<table>
<thead>
<tr>
<th>Components</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 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td>Remarks</td>
<td></td>
<td></td>
<td>Upper Respiratory Tract irritation</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>300 ppm 1,450 mg/m3</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>375 ppm 1,800 mg/m3</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>500 ppm 2,350 mg/m3</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
</tbody>
</table>

The value in mg/m3 is approximate.

<table>
<thead>
<tr>
<th>Components</th>
<th>Value</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>TWA</td>
<td>75 ppm 350 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td>C</td>
<td>385 ppm 1,800 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
</tbody>
</table>

15 minute ceiling value
Personal protective equipment

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).

Hand 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.

Immersion protection
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: > 480 min
Material tested: Camatri® (Aldrich Z677442, Size M)

Splash protection
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: > 30 min
Material tested: Dermatril® (Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 873000, 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 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.

Eye 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 and 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.

Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance
Form liquid
Colour colourless

Safety data
pH no data available
Melting point/range: -57 °C (-71 °F) - lit.
Boiling point 125 - 127 °C (257 - 261 °F) - lit.
Flash point 13.0 °C (55.4 °F) - closed cup
Ignition temperature 220 °C (428 °F)
Autoignition temperature 220.0 °C (428.0 °F)
Lower explosion limit 0.96 %(V)
Upper explosion limit 6.5 % (V)
Vapour pressure 14.7 hPa (11.0 mmHg) at 20.0 °C (68.0 °F)
Density 0.703 g/cm³ at 25 °C (77 °F)
Water solubility ca.0.007 g/l at 20 °C (68 °F)
Partition coefficient: n-octanol/water log Pow: 5.15
Relative vapour density no data available
Odour characteristic
Odour Threshold no data available
Evaporation rate no data available

10. STABILITY AND REACTIVITY

Chemical stability
Stable under recommended storage conditions.

Possibility of hazardous reactions
Vapours may form explosive mixture with air.

Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

Materials to avoid
Strong acids, Strong oxidizing agents

Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity
Oral LD50
Inhalation LC50
LC50 Inhalation - rat - 4 h - 118,000 mg/m³

Dermal LD50
no data available

Other information on acute toxicity
no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitization
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

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)
May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure (Globally Harmonized System)
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.

Potential health effects

<table>
<thead>
<tr>
<th>Exposure</th>
<th>Effect</th>
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<td>May cause eye irritation.</td>
</tr>
</tbody>
</table>

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

Synergistic effects
no data available

Additional Information
RTECS: RG8400000

12. ECOLOGICAL INFORMATION

Toxicity

<table>
<thead>
<tr>
<th>Taxonomy</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toxicity to fish</td>
<td>Mortality LC50 - Oryzias latipes - 0.42 mg/l - 96.0 h</td>
</tr>
<tr>
<td>Toxicity to daphnia and other aquatic invertebrates</td>
<td>Immobilization EC50 - Daphnia magna (Water flea) - 0.38 mg/l - 48 h</td>
</tr>
<tr>
<td>Toxicity to algae</td>
<td>Growth inhibition NOEC - Pseudokirchneriella subcapitata - 5.8 mg/l - 72 h</td>
</tr>
</tbody>
</table>

Persistence and degradability
no data available

Bioaccumulative potential
no data available

Mobility in soil
no data available

PBT and vPvB assessment
no data available

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

13. DISPOSAL CONSIDERATIONS

**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  
- Packing group: II  
- Proper shipping name: Octanes  
- Marine pollutant: No  
- Poison Inhalation Hazard: No

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

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

15. REGULATORY INFORMATION

**OSHA Hazards**
Flammable liquid, Irritant

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

**SARA 313 Components**
SARA 313: 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**
- Octane  
  - CAS-No.: 111-65-9  
  - Revision Date: 2007-03-01

**Pennsylvania Right To Know Components**
- Octane  
  - CAS-No.: 111-65-9  
  - Revision Date: 2007-03-01

**New Jersey Right To Know Components**
- Octane  
  - CAS-No.: 111-65-9  
  - Revision Date: 2007-03-01

**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

**Further information**
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