1. PRODUCT AND COMPANY IDENTIFICATION

Product name: Octane
Product Number: 296988
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 #: (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

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

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.
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**
- \( \text{C}_8\text{H}_{18} \)

**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>
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<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>
</tbody>
</table>

Remarks
Upper Respiratory Tract irritation

<table>
<thead>
<tr>
<th></th>
<th>TWA</th>
<th>Value</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>300 ppm</td>
<td>1,450 mg/m³</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<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>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.

15 minute ceiling value

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

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/freezing point 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

- **Inhalation**: May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.
- **Ingestion**: May be harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.
- **Skin**: May be harmful if absorbed through skin. May cause skin irritation.
- **Eyes**: May cause eye irritation.

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**
- **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 - 5.8 mg/l - 72 h

**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**
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life.

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

**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

**Massachusetts Right To Know Components**

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**Pennsylvania Right To Know Components**

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**New Jersey Right To Know Components**

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**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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