SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: Octane
Product Number: 296988
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 Inc.
3050 SPRUCE ST
ST. LOUIS MO  63103
UNITED STATES
Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 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
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (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

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**Signal word**

**Danger**

**Hazard statement(s)**

- **H225** Highly flammable liquid and vapor.
- **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/ vapors/ 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/ doctor.
- **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/ doctor 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**

**SECTION 3: Composition/information on ingredients**

**3.1 Substances**

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>n-Octane</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Formula</strong></td>
<td>C₈H₁₈</td>
</tr>
<tr>
<td><strong>Molecular weight</strong></td>
<td>114.23 g/mol</td>
</tr>
<tr>
<td><strong>CAS-No.</strong></td>
<td>111-65-9</td>
</tr>
<tr>
<td><strong>EC-No.</strong></td>
<td>203-892-1</td>
</tr>
<tr>
<td><strong>Index-No.</strong></td>
<td>601-009-00-8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
</table>

Sigma-Aldrich - 296988
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Call in physician.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

In case of eye contact
After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Carbon dioxide (CO2) Foam Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

For the full text of the H-Statements mentioned in this Section, see Section 16.
5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **Further information**
Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

**SECTION 6: Accidental release measures**

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains. Risk of explosion.

6.3 **Methods and materials for containment and cleaning up**
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 **Reference to other sections**
For disposal see section 13.

---

**SECTION 7: Handling and storage**

7.1 **Precautions for safe handling**

**Advice on safe handling**
Avoid generation of vapors/aerosols.

**Advice on protection against fire and explosion**
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

**Hygiene measures**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**

**Storage conditions**
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

- 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
SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients 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>n-octane</td>
<td>111-65-9</td>
<td>TWA</td>
<td>75 ppm 350 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>385 ppm 1,800 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</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>
<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>PEL</td>
<td>300 ppm 1,450 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>375 ppm 1,800 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>300 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Body Protection
Flame retardant antistatic protective clothing.

Respiratory protection
required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure
Do not let product enter drains. Risk of explosion.
## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>a)</strong> Appearance</td>
<td>Form: liquid&lt;br&gt;Color: colorless</td>
</tr>
<tr>
<td><strong>b)</strong> Odor</td>
<td>characteristic</td>
</tr>
<tr>
<td><strong>c)</strong> Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>d)</strong> pH</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>e)</strong> Melting point/freezing point</td>
<td>Melting point/range: -57 °C (-71 °F) - lit.</td>
</tr>
<tr>
<td><strong>f)</strong> Initial boiling point and boiling range</td>
<td>125 - 127 °C 257 - 261 °F - lit.</td>
</tr>
<tr>
<td><strong>g)</strong> Flash point</td>
<td>13 °C (55 °F) - closed cup</td>
</tr>
<tr>
<td><strong>h)</strong> Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>i)</strong> Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>j)</strong> Upper/lower flammability or explosive limits</td>
<td>Upper explosion limit: 6.5 %(V)&lt;br&gt;Lower explosion limit: 0.96 %(V)</td>
</tr>
<tr>
<td><strong>k)</strong> Vapor pressure</td>
<td>14.7 hPa at 20.0 °C (68.0 °F)</td>
</tr>
<tr>
<td><strong>l)</strong> Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>m)</strong> Density</td>
<td>0.703 g/cm3 at 25 °C (77 °F) - lit.</td>
</tr>
<tr>
<td></td>
<td>Relative density</td>
</tr>
<tr>
<td><strong>n)</strong> Water solubility</td>
<td>ca.0.007 g/l at 20 °C (68 °F)</td>
</tr>
<tr>
<td><strong>o)</strong> Partition coefficient: n-octanol/water</td>
<td>log Pow: 5.15</td>
</tr>
<tr>
<td><strong>p)</strong> Autoignition temperature</td>
<td>220 °C (428 °F)</td>
</tr>
<tr>
<td><strong>q)</strong> Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>r)</strong> Viscosity</td>
<td>0.8 mm²/s at 20 °C (68 °F) -</td>
</tr>
<tr>
<td><strong>s)</strong> Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>t)</strong> Oxidizing properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

### 9.2 Other safety information

No data available

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature).
10.3 **Possibility of hazardous reactions**  
Violent reactions possible with:  
Strong oxidizing agents

10.4 **Conditions to avoid**  
Warming.

10.5 **Incompatible materials**  
various plastics, Strong oxidizing agents

10.6 **Hazardous decomposition products**  
In the event of fire: see section 5

---

**SECTION 11: Toxicological information**

11.1 **Information on toxicological effects**

**Acute toxicity**  
LD50 Oral - Rat - male and female - > 5,000 mg/kg  
(OECD Test Guideline 401)  
Remarks: (in analogy to similar compounds)  
The value is given in analogy to the following substances: isoctane

LC50 Inhalation - Rat - male and female - 4 h - > 24.88 mg/l  
(OECD Test Guideline 403)  
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg  
(OECD Test Guideline 402)  
Remarks: (in analogy to similar products)  
The value is given in analogy to the following substances: isoctane

**Skin corrosion/irritation**  
Skin - Rabbit  
Result: Irritating to skin. - 24 h  
(OECD Test Guideline 404)  
Remarks: (in analogy to similar products)  
The value is given in analogy to the following substances: isoctane

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)  
Drying-out effect resulting in rough and chapped skin.

**Serious eye damage/eye irritation**  
Eyes - Rabbit  
Result: No eye irritation  
(OECD Test Guideline 405)  
Remarks: (in analogy to similar products)  
The value is given in analogy to the following substances: isoctane

**Respiratory or skin sensitization**  
Maximization Test - Guinea pig  
Result: negative  
(OECD Test Guideline 406)  
Remarks: (in analogy to similar products)

**Germ cell mutagenicity**  
Test Type: Ames test  
Test system: Escherichia coli/Salmonella typhimurium  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 471
Result: negative
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: n-heptane
Test Type: Chromosome aberration test in vitro
Test system: rat hepatocytes
Method: OECD Test Guideline 473
Result: negative
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: n-heptane
Test Type: In vitro mammalian cell gene mutation test
Test system: human lymphoblastoid cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: isooctane

**Carcinogenicity**
IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP: No ingredient 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 on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
Inhalation - May cause drowsiness or dizziness. - Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
Aspiration may cause pulmonary edema and pneumonitis.

### 11.2 Additional Information

RTECS: RG8400000
burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Vomiting, Central nervous system depression, narcosis
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

After uptake of large quantities:

- Headache
- Dizziness
- Nausea
- Vomiting
- agitation
- somnolence
- Drowsiness
- Unconsciousness
- respiratory arrest
It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

Handle in accordance with good industrial hygiene and safety practice.

**SECTION 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**
  - static test EC50 - Daphnia magna (Water flea) - 0.38 mg/l - 48 h
  - Remarks: (ECHA)
- **Toxicity to algae**
  - Growth inhibition NOEC - Pseudokirchneriella subcapitata (microalgae) - 5.8 mg/l - 72 h

**12.2 Persistence and degradability**

- **Biodegradability**
  - aerobic - Exposure time 10 d
  - Result: 70.3 % - Readily biodegradable.
  - Remarks: (ECHA)
  - Theoretical oxygen demand 3,500 mg/g
  - Remarks: (Lit.)

**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**

No data available

---

**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**

**Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.
SECTION 14: Transport information

DOT (US)
UN number: 1262  Class: 3  Packing group: II
Proper shipping name: Octanes
Reportable Quantity (RQ):
1) Marine pollutant: yes 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: yes
Marine pollutant: yes

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

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

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
No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information

Further information
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.

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