

FSHO3980

## Octane (Reagent)

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

**产品说明:**  
**Product Description:** 正辛烷  
 Octane (Reagent)

**Cat No. :** O3980-1  
**Synonyms** n-Octane.  
**CAS No** 111-65-9  
**Molecular Formula** C<sub>8</sub>H<sub>18</sub>

**Supplier** Fisher Scientific Company  
 One Reagent Lane  
 Fair Lawn, NJ 07410  
 Tel: (201) 796-7100

**Emergency Telephone Number** CHEMTREC®, Inside the USA: 800-424-9300  
 CHEMTREC®, Outside the USA: 001-703-527-3887

**E-mail address** begel.sdsdesk@thermofisher.com

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
 Liquid

**Appearance**  
 Clear

**Odor**  
 Petroleum distillates

#### Emergency Overview

Highly flammable liquid and vapor. May be fatal if swallowed and enters airways. Causes skin irritation. May cause drowsiness and dizziness. Very toxic to aquatic life with long lasting effects.

#### Classification of the substance or mixture

|  |            |
|--|------------|
| Flammable liquids.                                 | Category 2 |
| Aspiration Toxicity                                | Category 1 |
| Skin Corrosion/Irritation                          | Category 2 |
| Specific target organ toxicity - (single exposure) | Category 3 |
| Acute aquatic toxicity                             | Category 1 |
| Chronic aquatic toxicity                           | Category 1 |

#### Label Elements



**Signal Word****Danger****Hazard Statements**

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 Statements****Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
P240 - Ground and bond container and receiving equipment  
P242 - Use non-sparking tools  
P243 - Take action to prevent static discharges  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor  
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P331 - Do NOT induce vomiting  
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish  
P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

Vapors may cause flash fire or explosion. Highly flammable.

**Health Hazards**

Aspiration hazard if swallowed - can enter lungs and cause damage. Causes skin irritation. May cause drowsiness or dizziness.

**Environmental hazards**

Very toxic to aquatic life with long lasting effects. . Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil. The product is insoluble and floats on water.

**Other Hazards**

This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

| Component | CAS No   | Weight % |
|-----------|----------|----------|
| Octane    | 111-65-9 | > 95     |

**SECTION 4. FIRST AID MEASURES****General Advice**

If symptoms persist, call a physician.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs (by aspiration).

**Ingestion**

Clean mouth with water and drink afterwards plenty of water. Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.

**Most important symptoms and effects**

Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically. Symptoms may be delayed.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

**Extinguishing media which must not be used for safety reasons**

Do not use a solid water stream as it may scatter and spread fire.

**Specific Hazards Arising from the Chemical**

Flammable. Risk of ignition. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Thermal decomposition can lead to release of irritating gases and vapors. Keep product and empty container away from heat and sources of ignition. Vapors may form explosive mixtures with air. Do not allow run-off from fire-fighting to enter drains or water courses.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Use personal protective equipment as required. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

**Environmental Precautions**

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE**

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**Handling**

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded.

**Storage**

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame. Flammables area.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters**

| Component | China                      | Taiwan                                      | Thailand     | Hong Kong  |
|-----------|----------------------------|---|--------------|--|
| Octane    | TWA: 500 mg/m <sup>3</sup> | TWA: 300 ppm<br>TWA: 1400 mg/m <sup>3</sup> | TWA: 500 ppm | TWA: 300 ppm<br>TWA: 1400 mg/m <sup>3</sup><br>STEL: 375 ppm<br>STEL: 1750 mg/m <sup>3</sup> |

| Component | ACGIH TLV    | OSHA PEL  | NIOSH  | The United Kingdom | European Union |
|-----------|--------------|---|--|--------------------|----------------|
| Octane    | TWA: 300 ppm | (Vacated) TWA: 300 ppm<br>(Vacated) TWA: 1450 mg/m <sup>3</sup><br>(Vacated) STEL: 375 ppm<br>(Vacated) STEL: 1800 mg/m <sup>3</sup><br>TWA: 500 ppm<br>TWA: 2350 mg/m <sup>3</sup> | IDLH: 1000 ppm<br>TWA: 75 ppm<br>TWA: 350 mg/m <sup>3</sup><br>Ceiling: 385 ppm<br>Ceiling: 1800 mg/m <sup>3</sup> | -                  |                |

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

**Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

**Exposure Controls****Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment****Eye Protection**

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

**Hand Protection**

Protective gloves

| Glove material | Breakthrough time                 | Glove thickness | EU standard | Glove comments        |
|----------------|-----------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers recommendations | -               | EN 374      | (minimum requirement) |
| Viton (R)      |                                   |                 |             |                       |

Inspect gloves before use.

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Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.  
(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

|  |   |
|--|---|
| <b>Skin and body protection</b>        | Long sleeved clothing   |
| <b>Respiratory Protection</b>          | When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.<br>To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly   |
| <b>Large scale/emergency use</b>       | Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced<br><b>Recommended Filter type:</b> Organic gases and vapours filter Type A Brown conforming to EN14387  |
| <b>Small scale/Laboratory use</b>      | Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.<br><b>Recommended half mask:-</b> Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141<br>When RPE is used a face piece Fit Test should be conducted |
| <b>Hygiene Measures</b>                | Handle in accordance with good industrial hygiene and safety practice.  |
| <b>Environmental exposure controls</b> | Prevent product from entering drains. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained.   |

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

|  |                                 |   |
|--|---------------------------------|---|
| <b>Appearance</b>                              | Clear                           |   |
| <b>Physical State</b>                          | Liquid                          |   |
| <b>Odor</b>                                    | Petroleum distillates           |   |
| <b>Odor Threshold</b>                          | No data available               |   |
| <b>pH</b>                                      | No information available        |   |
| <b>Melting Point/Range</b>                     | -57 °C / -70.6 °F               |   |
| <b>Softening Point</b>                         | No data available               |   |
| <b>Boiling Point/Range</b>                     | 124 - 127 °C / 255.2 - 260.6 °F |   |
| <b>Flash Point</b>                             | 13 °C / 55.4 °F                 | <b>Method -</b> No information available    |
| <b>Evaporation Rate</b>                        | 0.6 (Butyl Acetate = 1.0)       |   |
| <b>Flammability (solid,gas)</b>                | Not applicable                  | Liquid                                      |
| <b>Explosion Limits</b>                        | No data available               |   |
| <b>Vapor Pressure</b>                          | 11 mmHg @ 20 °C                 |   |
| <b>Vapor Density</b>                           | 3.9 (Air = 1.0)                 | (Air = 1.0)                                 |
| <b>Specific Gravity / Density</b>              | 0.708                           |   |
| <b>Bulk Density</b>                            | Not applicable                  | Liquid                                      |
| <b>Water Solubility</b>                        | Insoluble                       |   |
| <b>Solubility in other solvents</b>            | No information available        |   |
| <b>Partition Coefficient (n-octanol/water)</b> |                                 |   |
| <b>Component</b>                               | <b>log Pow</b>                  |   |
| Octane   | 5.18                            |   |
| <b>Autoignition Temperature</b>                | 206 - °C / 402.8 - °F           |   |
| <b>Decomposition Temperature</b>               | No data available               |   |
| <b>Viscosity</b>                               | No data available               |   |
| <b>Explosive Properties</b>                    |                                 | Vapors may form explosive mixtures with air |
| <b>Oxidizing Properties</b>                    | No information available        |   |

## Octane (Reagent)

Molecular Formula C<sub>8</sub>H<sub>18</sub>  
Molecular Weight 114.23  
VOC Content(%) 95

## SECTION 10. STABILITY AND REACTIVITY

**Stability** Stable under normal conditions.

**Hazardous Reactions** None under normal processing.

**Hazardous Polymerization** Hazardous polymerization does not occur.

**Conditions to Avoid** Keep away from open flames, hot surfaces and sources of ignition. Incompatible products. Excess heat.

**Materials to avoid** Strong oxidizing agents.

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

| Component | LD50 Oral     | LD50 Dermal      | LC50 Inhalation               |
|-----------|---------------|------------------|-------------------------------|
| Octane    | >5 g/kg (Rat) | >2 g/kg (Rabbit) | LC50 > 24.88 mg/L ( Rat ) 4 h |

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; No data available

## (d) respiratory or skin sensitization;

Respiratory No data available  
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Central nervous system (CNS)

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Category 1

**Symptoms / effects, both acute and** Inhalation of high vapor concentrations may cause symptoms like headache, dizziness,

## Octane (Reagent)

delayed tiredness, nausea and vomiting

## SECTION 12. ECOLOGICAL INFORMATION

## Ecotoxicity effects

The product contains following substances which are hazardous for the environment. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

| Component | Freshwater Fish | Water Flea                             | Freshwater Algae | Microtox                  |
|-----------|-----------------|--|------------------|---------------------------|
| Octane    |                 | EC50: = 0.38 mg/L, 48h<br>(water flea) |                  | EC50 = 890 mg/L 30<br>min |

## Persistence and Degradability

## Persistence

May persist.

Degradation in sewage  
treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

## Bioaccumulative Potential

Product has a high potential to bioconcentrate

| Component | log Pow | Bioconcentration factor (BCF) |
|-----------|---------|-------------------------------|
| Octane    | 5.18    | No data available             |

## Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and floats on water Is not likely mobile in the environment due its low water solubility Is not likely mobile in the environment due its low water solubility and propensity to bind to soil particles

## Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

## Persistent Organic Pollutant

This product does not contain any known or suspected substance

## Ozone Depletion Potential

This product does not contain any known or suspected substance

## SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused  
Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

## Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

## Other Information

Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Can be landfilled or incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains.

## SECTION 14. TRANSPORT INFORMATION

## Road and Rail Transport

|                      |         |
|----------------------|---------|
| UN-No                | UN1262  |
| Proper Shipping Name | OCTANES |
| Hazard Class         | 3       |
| Packing Group        | II      |

## IMDG/IMO

**SAFETY DATA SHEET**

Revision Date 15-May-2024

Octane (Reagent)

**UN-No** UN1262  
**Proper Shipping Name** OCTANES  
**Hazard Class** 3  
**Packing Group** II

**IATA**

**UN-No** UN1262  
**Proper Shipping Name** OCTANES  
**Hazard Class** 3  
**Packing Group** II

**Special Precautions for User** No special precautions required

**SECTION 15. REGULATORY INFORMATION****International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

| Component | The Inventory of Hazardous Chemicals (2015 Edition) | List of dangerous goods GB 12268 - 2012 | TCSI | IECSC | EINECS    | TSCA | DSL | PICCS | ENCS | ISHL | AICS | KECL     |
|-----------|---|---|------|-------|-----------|------|-----|-------|------|------|------|----------|
| Octane    | X   | X                                       | X    | X     | 203-892-1 | X    | X   | X     | X    | X    | X    | KE-26612 |

**National Regulations****SECTION 16. OTHER INFORMATION**

**Creation Date** 07-Oct-2014  
**Revision Date** 15-May-2024  
**Revision Summary** Not applicable.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.

Chemical incident response training.

**Legend**

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer



## Octane (Reagent)

**DNEL** - Derived No Effect Level  
**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**PNEC** - Predicted No Effect Concentration  
**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association  
**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**OECD** - Organisation for Economic Co-operation and Development  
**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code  
**MARPOL** - International Convention for the Prevention of Pollution from Ships  
**ATE** - Acute Toxicity Estimate  
**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**