Material Safety Data Sheet
Isooctane

ACC# 28270

Section 1 - Chemical Product and Company Identification

**MSDS Name:** Isooctane  
**Catalog Numbers:** AC167910000, AC167910025, AC167915000, AC265440000, AC265440010, AC265440025, AC268810000, AC268810010, AC268810025, AC295720000, AC295720010, AC295720025, AC326620000, AC326620010, AC326620025, AC326940000, AC326941000, AC326942500, AC364670000, AC364671000, AC412710000, AC412711000, AC421970000, AC421970020, AC421970200, AC421970250, AC421975000, AC421980000, AC421980040, AC421985000, AC424560000, AC424560010, AC424565000, AC610120040, AC610210040, NC9809854, O296-1, O296-4, O296J4, O296RS115, O296RS28, O296SK-1, O296SK-4, O296SS115, O296SS200, O296SS28, O296SS50, O297-4, O299-1, O299-4, O299FB200, O299FB50, O299J1, O299RS115, O299SS115, O299SS200, O299SS28, O299SS50, O300-1, O300-4, O301-1, O301-4  
**Synonyms:** Isooctane; Isobutyltrimethylmethane; 2,4,4-Trimethylpentane.  
**Company Identification:**  
Fisher Scientific  
1 Reagent Lane  
Fair Lawn, NJ 07410  
For information, call: 201-796-7100  
Emergency Number: 201-796-7100  
For CHEMTREC assistance, call: 800-424-9300  
For International CHEMTREC assistance, call: 703-527-3887

Section 2 - Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>CAS#</th>
<th>Chemical Name</th>
<th>Percent</th>
<th>EINECS/ELINCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>540-84-1</td>
<td>Isooctane</td>
<td>&gt;95</td>
<td>208-759-1</td>
</tr>
</tbody>
</table>

Section 3 - Hazards Identification

**EMERGENCY OVERVIEW**

Appearance: clear, colorless liquid. Flash Point: -12 deg C.  
**Danger!** Extremely flammable liquid and vapor. Vapor may cause flash fire. Breathing vapors may cause drowsiness and dizziness. Causes eye, skin, and respiratory tract irritation. Aspiration hazard if swallowed. Can enter lungs and cause damage.  
**Target Organs:** Central nervous system, lungs, eyes, skin.

**Potential Health Effects**  
**Eye:** Causes eye irritation. Causes redness and pain. Exposure to high vapor concentrations may cause irritation.  
**Skin:** Causes skin irritation. Prolonged and/or repeated contact may cause defatting of the skin and dermatitis. A single prolonged skin exposure is not likely to result in the material being absorbed in harmful amounts.  
**Ingestion:** May cause gastrointestinal irritation with nausea, vomiting and diarrhea. Aspiration of material into the lungs may cause chemical pneumonitis, which may be fatal. May cause central nervous system depression.  
**Inhalation:** Causes respiratory tract irritation. May cause narcotic effects in high concentration. Aspiration may lead to pulmonary edema.  
**Chronic:** Prolonged or repeated skin contact may cause defatting and dermatitis. In a subchronic
oral laboratory study, isooctane produced kidney damage in male rats only. No comparable health hazard for kidney disease is known to occur in

Section 4 - First Aid Measures

**Eyes:** In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical aid.

**Skin:** In case of contact, immediately flush skin with plenty of water. Remove contaminated clothing and shoes. Get medical aid. Wash clothing before reuse.

**Ingestion:** Potential for aspiration if swallowed. Get medical aid immediately. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If vomiting occurs naturally, have victim lean forward.

**Inhalation:** If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.

**Notes to Physician:** Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

**General Information:** As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Liquid will float and may reignite on the surface of water. Extremely flammable liquid and vapor. Vapor may cause flash fire. Vapors are heavier than air and may travel to a source of ignition and flash back. Vapors can spread along the ground and collect in low or confined areas. May accumulate static electricity.

**Extinguishing Media:** Water may be ineffective. This material is lighter than water and insoluble in water. The fire could easily be spread by the use of water in an area where the water cannot be contained. Do NOT use straight streams of water. Dry chemical, alcohol foam, carbon dioxide.

**Flash Point:** -12 deg C (10.40 deg F)

**Autoignition Temperature:** 415 deg C (779.00 deg F)

**Explosion Limits, Lower:** 1.1%

**Upper:** 6.0%

**NFPA Rating:** (estimated) Health: 1; Flammability: 3; Instability: 0

Section 6 - Accidental Release Measures

**General Information:** Use proper personal protective equipment as indicated in Section 8.

**Spills/Leaks:** Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Avoid runoff into storm sewers and ditches which lead to waterways. Remove all sources of ignition. Use a spark-proof tool. Provide ventilation. A vapor suppressing foam may be used to reduce vapors.

Section 7 - Handling and Storage

**Handling:** Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Ground and bond containers when transferring material. Use spark-proof tools and explosion proof equipment. Avoid contact with eyes, skin, and clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Take precautionary measures against static discharges. Keep container tightly closed. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames. Use only with adequate ventilation. Keep away from heat, sparks and flame. Avoid breathing vapor or mist.

**Storage:** Keep away from sources of ignition. Store in a tightly closed container. Keep from contact with oxidizing materials. Store in a cool, dry, well-ventilated area away from incompatible substances. Flammables-area.
Section 8 - Exposure Controls, Personal Protection

**Engineering Controls:** Use process enclosure, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Ventilation fans and other electrical service must be non-sparking and have an explosion-proof design.

**Exposure Limits**

<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>ACGIH</th>
<th>NIOSH</th>
<th>OSHA - Final PELs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isooctane</td>
<td>300 ppm TWA (listed under Octane).</td>
<td>75 ppm TWA; 350 mg/m³ TWA (listed under Octane). 1000 ppm IDLH (listed under Octane).</td>
<td>500 ppm TWA; 2350 mg/m³ TWA (listed under Octane).</td>
</tr>
</tbody>
</table>

**OSHA Vacated PELs:** Isooctane: No OSHA Vacated PELs are listed for this chemical.

**Personal Protective Equipment**

**Eyes:** Wear chemical splash goggles.

**Skin:** Wear appropriate gloves to prevent skin exposure.

**Clothing:** Wear appropriate protective clothing to prevent skin exposure.

**Respirators:** A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use.

Section 9 - Physical and Chemical Properties

**Physical State:** Liquid

**Appearance:** clear, colorless

**Odor:** gasoline-like

**pH:** Not applicable.

**Vapor Pressure:** 49.3 mm Hg @ 25 deg C

**Vapor Density:** 3.94 (air=1)

**Evaporation Rate:** < 1 (ether=1)

**Viscosity:** 0.51 mPas 22 deg C

**Boiling Point:** 98 - 99 deg C @ 760 mmHg

**Freezing/Melting Point:** -107 deg C

**Decomposition Temperature:** Not available.

**Solubility:** insoluble

**Specific Gravity/Density:** 0.69 g/cm³

**Molecular Formula:** C₈H₁₈

**Molecular Weight:** 114.23

Section 10 - Stability and Reactivity

**Chemical Stability:** Stable at room temperature in closed containers under normal storage and handling conditions.

**Conditions to Avoid:** Ignition sources, excess heat, electrical sparks, confined spaces.

**Incompatibilities with Other Materials:** Strong oxidizing agents, strong acids, strong bases.

**Hazardous Decomposition Products:** Carbon monoxide, carbon dioxide.

**Hazardous Polymerization:** Will not occur.

Section 11 - Toxicological Information

RTECS#: 

CAS# 540-84-1: SA3320000
LD50/LC50:
Not available.
Dermal LD50 (rabbit): >2000 mg/kg; Inhalation LC50 (rat): >3078.44 ppm/4H; Oral LD50 (rat) :>5000 mg/kg (values from Phillips 66).
Carcinogenicity:
CAS# 540-84-1: Not listed by ACGIH, IARC, NTP, or CA Prop 65.
Epidemiology: Not available.
Teratogenicity: Not available.
Reproductive Effects: Not available.
Mutagenicity: See actual entry in RTECS for complete information.
Neurotoxicity: Not available.
Other Studies:

Section 12 - Ecological Information
No information available.

Section 13 - Disposal Considerations
Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.
RCRA P-Series: None listed.
RCRA U-Series: None listed.

Section 14 - Transport Information

<table>
<thead>
<tr>
<th></th>
<th>US DOT</th>
<th>Canada TDG</th>
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<tbody>
<tr>
<td>Shipping Name:</td>
<td>OCTANES</td>
<td>OCTANES</td>
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<tr>
<td>Hazard Class:</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>UN Number:</td>
<td>UN1262</td>
<td>UN1262</td>
</tr>
<tr>
<td>Packing Group:</td>
<td>II</td>
<td>II</td>
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</tbody>
</table>

Section 15 - Regulatory Information

US FEDERAL

TSCA
CAS# 540-84-1 is listed on the TSCA inventory.

Health & Safety Reporting List
CAS# 540-84-1: Effective 6/1/87, Sunset 12/19/95

Chemical Test Rules
None of the chemicals in this product are under a Chemical Test Rule.

Section 12b
None of the chemicals are listed under TSCA Section 12b.

TSCA Significant New Use Rule
None of the chemicals in this material have a SNUR under TSCA.

CERCLA Hazardous Substances and corresponding RQs
CAS# 540-84-1: 1000 lb final RQ; 454 kg final RQ

SARA Section 302 Extremely Hazardous Substances
None of the chemicals in this product have a TPQ.

SARA Codes
CAS # 540-84-1: immediate, fire.

Section 313  No chemicals are reportable under Section 313.

Clean Air Act:  
CAS# 540-84-1 is listed as a hazardous air pollutant (HAP).  
This material does not contain any Class 1 Ozone depletors.  
This material does not contain any Class 2 Ozone depletors.

Clean Water Act:  
None of the chemicals in this product are listed as Hazardous Substances under the CWA.  
None of the chemicals in this product are listed as Priority Pollutants under the CWA.  
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:  
None of the chemicals in this product are considered highly hazardous by OSHA.

STATE  
CAS# 540-84-1 can be found on the following state right to know lists: California, (listed as Octane), New Jersey, Pennsylvania, Minnesota, (listed as Octane), Massachusetts.

California Prop 65  
California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations  
European Labeling in Accordance with EC Directives

Hazard Symbols:
XN F N

Risk Phrases:  
R 11 Highly flammable.  
R 38 Irritating to skin.  
R 50/53 Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.  
R 65 Harmful: may cause lung damage if swallowed.  
R 67 Vapours may cause drowsiness and dizziness.

Safety Phrases:  
S 16 Keep away from sources of ignition - No smoking.  
S 29 Do not empty into drains.  
S 33 Take precautionary measures against static discharges.  
S 9 Keep container in a well-ventilated place.  
S 60 This material and its container must be disposed of as hazardous waste.  
S 61 Avoid release to the environment. Refer to special instructions /safety data sheets.  
S 62 If swallowed, do not induce vomiting: seek medical advice immediately and show this container or label.

WGK (Water Danger/Protection)  
CAS# 540-84-1: No information available.

Canada - DSL/NDSL  
CAS# 540-84-1 is listed on Canada's DSL List.

Canada - WHMIS  
This product has a WHMIS classification of B2, D2B. This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List  
CAS# 540-84-1 (listed as Octane) is listed on the Canadian Ingredient Disclosure List.

Section 16 - Additional Information

MSDS Creation Date: 12/12/1997  
Revision #14 Date: 6/06/2006

The information above is believed to be accurate and represents the best information currently available to us. However, we
make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall Fisher be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if Fisher has been advised of the possibility of such damages.