



Neutron<sup>®</sup>Pharmachemical Co.  
Manufacturer of Laboratory Chemical & Pharmaceutical Materials

# SAFETY DATA SHEET

Creation Date 22-Jun-2009

Revision Date 17-Jan-2018

Revision Number 5

## 1. Identification

**Product Name** Isooctane

**Cat No. :** 3.3000

**CAS-No** 540-84-1  
**Synonyms** Isooctane

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Not for food, drug, pesticide or biocidal product use

### Details of the supplier of the safety data sheet

#### Company

NEUTRON PHARMACHEMICAL CO  
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#### **Emergency Telephone Number**

CHEMTREC<sup>®</sup>, 125

## 2. Hazard(s) identification

### Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

|  |            |
|--|------------|
| Flammable liquids                                | Category 2 |
| Skin Corrosion/irritation                        | Category 2 |
| Serious Eye Damage/Eye Irritation                | Category 2 |
| Specific target organ toxicity (single exposure) | Category 3 |
| Target Organs - Central nervous system (CNS).    |            |
| Aspiration Toxicity                              | Category 1 |

### Label Elements

#### **Signal Word**

Danger

#### **Hazard Statements**

Highly flammable liquid and vapor  
May be fatal if swallowed and enters airways  
Causes skin irritation  
Causes serious eye irritation  
May cause drowsiness or dizziness

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling  
 Wear protective gloves/protective clothing/eye protection/face protection  
 Do not breathe dust/fume/gas/mist/vapors/spray  
 Use only outdoors or in a well-ventilated area  
 Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
 Keep container tightly closed  
 Ground/bond container and receiving equipment  
 Use explosion-proof electrical/ventilating/lighting/equipment  
 Use only non-sparking tools  
 Take precautionary measures against static discharge  
 Keep cool

**Response**

Get medical attention/advice if you feel unwell

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
 Call a POISON CENTER or doctor/physician if you feel unwell

**Skin**

If skin irritation occurs: Get medical advice/attention  
 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower  
 Wash contaminated clothing before reuse

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
 If eye irritation persists: Get medical advice/attention

**Ingestion**

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
 Do NOT induce vomiting

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam for extinction

**Storage**

Store locked up  
 Store in a well-ventilated place. Keep container tightly closed

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

Very toxic to aquatic life with long lasting effects

### 3. Composition/Information on Ingredients

| Component | CAS-No   | Weight % |
|-----------|----------|----------|
| Isooctane | 540-84-1 | >95      |

### 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.

|  |   |
|--|---|
| <b>Skin Contact</b>                        | Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.   |
| <b>Inhalation</b>                          | Move to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. Risk of serious damage to the lungs.   |
| <b>Ingestion</b>                           | 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. |
| <b>Most important symptoms and effects</b> | None reasonably foreseeable. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting  |
| <b>Notes to Physician</b>                  | Treat symptomatically   |

## 5. Fire-fighting measures

|   |   |
|---|---|
| <b>Suitable Extinguishing Media</b>     | Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray. |
| <b>Unsuitable Extinguishing Media</b>   | Water may be ineffective, Do not use a solid water stream as it may scatter and spread fire                                       |
| <b>Flash Point</b>                      | -12 °C / 10.4 °F  |
| <b>Method -</b>                         | No information available  |
| <b>Autoignition Temperature</b>         | 410 °C / 770 °F   |
| <b>Explosion Limits</b>                 |   |
| <b>Upper</b>                            | 6.0 vol %   |
| <b>Lower</b>                            | 1.1 vol %   |
| <b>Sensitivity to Mechanical Impact</b> | No information available  |
| <b>Sensitivity to Static Discharge</b>  | No information available  |

### 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. Vapors may form explosive mixtures with air. Do not allow run-off from fire fighting to enter drains or water courses.

### Hazardous Combustion Products

Carbon monoxide (CO) Carbon dioxide (CO<sub>2</sub>)

### 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.

### NFPA

|               |                     |                    |                         |
|---------------|---------------------|--------------------|-------------------------|
| <b>Health</b> | <b>Flammability</b> | <b>Instability</b> | <b>Physical hazards</b> |
| 3             | 3                   | 0                  | N/A                     |

## 6. Accidental release measures

|   |   |
|---|---|
| <b>Personal Precautions</b>                 | Use personal protective equipment. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.  |
| <b>Environmental Precautions</b>            | 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. |
| <b>Methods for Containment and Clean Up</b> | Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.   |

## 7. Handling and storage

|                 |   |
|-----------------|---|
| <b>Handling</b> | Wear personal protective equipment. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges. |
| <b>Storage</b>  | Keep away from open flames, hot surfaces and sources of ignition. Keep containers tightly closed in a dry, cool and well-ventilated place. Flammables area. Keep away from heat and sources of ignition.  |

## 8. Exposure controls / personal protection

### Exposure Guidelines

| Component | ACGIH TLV    | OSHA PEL | NIOSH IDLH | Mexico OEL (TWA) |
|-----------|--------------|----------|------------|------------------|
| Isooctane | TWA: 300 ppm |          |            |                  |

### Legend

ACGIH - American Conference of Governmental Industrial Hygienists

|                             |   |
|-----------------------------|---|
| <b>Engineering Measures</b> | Use only under a chemical fume hood. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. |
|-----------------------------|---|

### Personal Protective Equipment

|                                 |   |
|---------------------------------|---|
| <b>Eye/face Protection</b>      | Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.   |
| <b>Skin and body protection</b> | Long sleeved clothing.  |
| <b>Respiratory Protection</b>   | Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. |
| <b>Hygiene Measures</b>         | Handle in accordance with good industrial hygiene and safety practice.  |

## 9. Physical and chemical properties

|   |  |
|---|--|
| <b>Physical State</b>                         | Liquid                                   |
| <b>Appearance</b>                             | Colorless                                |
| <b>Odor</b>                                   | Petroleum distillates                    |
| <b>Odor Threshold</b>                         | No information available                 |
| <b>pH</b>                                     | Not applicable                           |
| <b>Melting Point/Range</b>                    | -107 °C / -160.6 °F                      |
| <b>Boiling Point/Range</b>                    | 98 - 99 °C / 208.4 - 210.2 °F @ 760 mmHg |
| <b>Flash Point</b>                            | -12 °C / 10.4 °F                         |
| <b>Evaporation Rate</b>                       | No information available                 |
| <b>Flammability (solid,gas)</b>               | Not applicable                           |
| <b>Flammability or explosive limits</b>       |  |
| Upper   | 6.0 vol %                                |
| Lower   | 1.1 vol %                                |
| <b>Vapor Pressure</b>                         | 51 mbar @ 20 °C                          |
| <b>Vapor Density</b>                          | 3.94                                     |
| <b>Specific Gravity</b>                       | 0.690                                    |
| <b>Solubility</b>                             | immiscible                               |
| <b>Partition coefficient; n-octanol/water</b> | No data available                        |
| <b>Autoignition Temperature</b>               | 410 °C / 770 °F                          |

|                                  |                          |
|----------------------------------|--------------------------|
| <b>Decomposition Temperature</b> | No information available |
| <b>Viscosity</b>                 | 0.51 mPa s at 22 °C      |
| <b>Molecular Formula</b>         | C8 H18                   |
| <b>Molecular Weight</b>          | 114.23                   |

## 10. Stability and reactivity

|   |   |
|---|---|
| <b>Reactive Hazard</b>                  | None known, based on information available  |
| <b>Stability</b>                        | Stable under normal conditions.   |
| <b>Conditions to Avoid</b>              | Incompatible products. Heat, flames and sparks. Keep away from open flames, hot surfaces and sources of ignition. |
| <b>Incompatible Materials</b>           | Strong oxidizing agents, Strong acids, Strong bases   |
| <b>Hazardous Decomposition Products</b> | Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> )   |
| <b>Hazardous Polymerization</b>         | Hazardous polymerization does not occur.  |
| <b>Hazardous Reactions</b>              | None under normal processing.   |

## 11. Toxicological information

### Acute Toxicity

#### Product Information Component Information

| Component | LD50 Oral               | LD50 Dermal         | LC50 Inhalation               |
|-----------|-------------------------|---------------------|-------------------------------|
| Isooctane | LD50 5000 mg/kg ( Rat ) | 2000 mg/kg (Rabbit) | LC50 = 33.52 mg/L ( Rat ) 4 h |

**Toxicologically Synergistic Products** No information available

### Delayed and immediate effects as well as chronic effects from short and long-term exposure

|                        |  |
|------------------------|--|
| <b>Irritation</b>      | Irritating to eyes, respiratory system and skin  |
| <b>Sensitization</b>   | No information available   |
| <b>Carcinogenicity</b> | The table below indicates whether each agency has listed any ingredient as a carcinogen. |

| Component | CAS-No   | IARC       | NTP        | ACGIH      | OSHA       | Mexico     |
|-----------|----------|------------|------------|------------|------------|------------|
| Isooctane | 540-84-1 | Not listed | Not listed | Not listed | Not listed | Not listed |

|   |   |
|---|---|
| <b>Mutagenic Effects</b>                          | No information available  |
| <b>Reproductive Effects</b>                       | No information available.   |
| <b>Developmental Effects</b>                      | No information available.   |
| <b>Teratogenicity</b>                             | No information available.   |
| <b>STOT - single exposure</b>                     | Central nervous system (CNS)  |
| <b>STOT - repeated exposure</b>                   | None known  |
| <b>Aspiration hazard</b>                          | No information available  |
| <b>Symptoms / effects, both acute and delayed</b> | Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting |
| <b>Endocrine Disruptor Information</b>            | No information available  |

**Other Adverse Effects** The toxicological properties have not been fully investigated.

## 12. Ecological information

### Ecotoxicity

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

| Component | Freshwater Algae     | Freshwater Fish                           | Microtox   | Water Flea                             |
|-----------|----------------------|---|------------|--|
| Isooctane | EC50= 2.94 mg/l, 72h | LC50 = 0.11 mg/l, 96h,<br>(Rainbow trout) | Not listed | EC50= 0.4 mg/l, 48h<br>(Daphnia magna) |

**Persistence and Degradability** Insoluble in water Persistence is unlikely based on information available. Immiscible with water

**Bioaccumulation/ Accumulation** No information available.

**Mobility** Will likely be mobile in the environment due to its volatility. Is not likely mobile in the environment due its low water solubility.

## 13. Disposal considerations

**Waste Disposal Methods** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## 14. Transport information

### DOT

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

### TDG

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

### IMDG/IMO

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

## 15. Regulatory information

All of the components in the product are on the following Inventory lists: X = listed

### International Inventories

| Component | TSCA | DSL | NDSL | EINECS    | ELINCS | NLP | PICCS | ENCS | AICS | IECSC | KECL |
|-----------|------|-----|------|-----------|--------|-----|-------|------|------|-------|------|
| Isooctane | X    | X   | -    | 208-759-1 | -      |     | X     | X    | X    | X     | X    |

### Legend:

X - Listed

E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.

F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.

N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.

**P** - Indicates a commenced PMN substance  
**R** - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.  
**S** - Indicates a substance that is identified in a proposed or final Significant New Use Rule  
**T** - Indicates a substance that is the subject of a Section 4 test rule under TSCA.  
**XU** - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B)).  
**Y1** - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.  
**Y2** - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

**U.S. Federal Regulations**

**TSCA 12(b)** Not applicable  
**SARA 313** Not applicable  
**SARA 311/312 Hazard Categories** See section 2 for more information  
**CWA (Clean Water Act)** Not applicable

**Clean Air Act**

| Component | HAPS Data | Class 1 Ozone Depletors | Class 2 Ozone Depletors |
|-----------|-----------|-------------------------|-------------------------|
| Isooctane | X         |                         | -                       |

**OSHA** Occupational Safety and Health Administration  
Not applicable

**CERCLA** This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302)

| Component | Hazardous Substances RQs | CERCLA EHS RQs |
|-----------|--------------------------|----------------|
| Isooctane | 1000 lb                  | -              |

**California Proposition 65** This product does not contain any Proposition 65 chemicals

**U.S. State Right-to-Know Regulations**

| Component | Massachusetts | New Jersey | Pennsylvania | Illinois | Rhode Island |
|-----------|---------------|------------|--------------|----------|--------------|
| Isooctane | X             | X          | X            | X        | -            |

**U.S. Department of Transportation**

Reportable Quantity (RQ): Y  
 DOT Marine Pollutant N  
 DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security**  
 This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** Serious risk, Grade 3

**16. Other information**

**Prepared By** Regulatory Affairs  
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**Revision Summary**

This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

**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 SDS**