



N-OCTANE-D18 (D, 99%)

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Issue date: 12/15/2010 Revision date: 3/2/2023 Supersedes: 1/7/2014 Version: 3.1

SECTION 1: Identification

1.1. Identification

Product form	: Substance
Substance name	: N-OCTANE-D18 (D, 99%)
Chemical name	: Octane
CAS-No.	: 111-65-9
Product code	: DLM-50
Formula	: C ₈ H ₁₈
Synonyms	: Octane

1.2. Recommended use and restrictions on use

No additional information available

1.3. Supplier

Cambridge Isotope Laboratories, Inc.
50 Frontage Rd
01810
ANDOVER, MA, 01810
USA
T 1-800-322-1174
cilsales@isotope.com - www.isotope.com

1.4. Emergency telephone number

Emergency number : 1-703-741-5970
Chemtrec 1-800-424-9300 24 hours

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Flammable liquids Category 2	H225	Highly flammable liquid and vapor
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Specific target organ toxicity – Single exposure, Category 3, Narcosis	H336	May cause drowsiness or dizziness
Aspiration hazard Category 1	H304	May be fatal if swallowed and enters airways
Hazardous to the aquatic environment – Acute Hazard Category 1	H400	Very toxic to aquatic life
Hazardous to the aquatic environment – Chronic Hazard Category 1	H410	Very toxic to aquatic life with long lasting effects
Full text of H statements : see section 16		

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US) :



Signal word (GHS US) :

Danger

Hazard statements (GHS US) :

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

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Precautionary statements (GHS US)

H400 - Very toxic to aquatic life
H410 - Very toxic to aquatic life with long lasting effects
: P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. heat, hot surfaces, open flames, sparks
P233 - Keep container tightly closed.
P240 - Ground/Bond container and receiving equipment.
P241 - Use explosion-proof electrical, lighting, ventilating equipment.
P242 - Use only non-sparking tools.
P243 - Take precautionary measures against static discharge.
P261 - Avoid breathing fume, mist, spray, vapors.
P264 - Wash Both hands thoroughly after handling.
P271 - Use only outdoors or in a well-ventilated area.
P273 - Avoid release to the environment.
P280 - Wear protective clothing, protective gloves.
P301+P310 - If swallowed: Immediately call a poison center or doctor.
P302+P352 - If on skin: Wash with plenty of water.
P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing.
P312 - Call a poison center or doctor if you feel unwell.
P321 - Specific treatment (see Hazard pictograms (CLP) on this label).
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 Alcohol resistant foam, Carbon dioxide, Dry powder, Water spray 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 Comply with applicable regulations.

2.3. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	GHS US classification
N-OCTANE-D18 (D, 99%) (Main constituent)	CAS-No.: 111-65-9	100	Flam. Liq. 2, H225 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

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SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general	: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
First-aid measures after inhalation	: If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
First-aid measures after skin contact	: Wash off with soap and plenty of water. Consult a physician.
First-aid measures after eye contact	: Flush eye with water for 15 minutes. Get medical attention.
First-aid measures after ingestion	: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2. Most important symptoms and effects (acute and delayed)

Potential Adverse human health effects and symptoms	: Burning sensation. Cough. Wheezing. Laryngitis. Shortness of breath. Headache. Nausea. Vomiting. Central nervous system depression. Narcosis.
Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.
Symptoms/effects after skin contact	: May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/effects after eye contact	: May cause eye irritation.
Symptoms/effects after ingestion	: Aspiration hazard if swallowed - can enter lungs and cause damage. May be harmful if swallowed.

4.3. Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media	: Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.
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5.2. Specific hazards arising from the chemical

No additional information available

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions	: Wear self contained breathing apparatus for fire fighting if necessary.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.
Other information	: Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures	: 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.
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6.1.2. For emergency responders

No additional information available

6.2. 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.

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6.3. Methods and material for containment and cleaning up

For containment : 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. Do not flush with water. Keep in suitable, closed containers for disposal.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent build up of electrostatic charge.

Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Keep container tightly closed in a cool, dry and well-ventilated place. Opened containers must be carefully resealed and kept upright to prevent leakage.

Storage conditions : Store at room temperature away from light and moisture.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

N-OCTANE-D18 (D, 99%) (111-65-9)	
USA - ACGIH - Occupational Exposure Limits	
Local name	Octane, all isomers
ACGIH OEL TWA [ppm]	300 ppm Upper Respiratory Tract irritation.
Remark (ACGIH)	TLV® Basis: URT irr
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
Regulatory reference	ACGIH 2022
USA - OSHA - Occupational Exposure Limits	
Local name	Octane
OSHA PEL TWA [1]	2350 The value in mg/m ³ is approximate.
OSHA PEL TWA [2]	500 ppm
Regulatory reference (US-OSHA)	OSHA Annotated Table Z-1
USA - NIOSH - Occupational Exposure Limits	
NIOSH REL TWA	350 mg/m ³
NIOSH REL TWA [ppm]	75 ppm
NIOSH REL C	1800 mg/m ³ 15 minute ceiling value.
NIOSH REL C [ppm]	385 ppm 15 minute ceiling value.

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8.2. Appropriate engineering controls

No additional information available

8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.

Eye protection:

Wear safety glasses with side shields (or goggles) and a face shield.

Skin and body protection:

Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Respiratory protection:

When appropriate, use NIOSH/CEN approved respirator.

Personal protective equipment symbol(s):



SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Liquid.
Color	: Colorless
Odor	: Characteristic
Odor threshold	: No data available
pH	: No data available
Melting point	: -56.73 °C Source: HSDB
Freezing point	: No data available
Boiling point	: 125.62 °C Source: HSDB
Flash point	: 13 °C Source: ECHA
Relative evaporation rate (butyl acetate=1)	: 1
Flammability (solid, gas)	: No data available
Vapor pressure	: 14.1 mm Hg at 25°C Source: HSDB
Relative vapor density at 20°C	: 3.86 Source: HSDB
Relative density	: 0.6986 Source: HSDB
Density	: 0.703 g/ml at 25 °C (77 °F)
Molecular mass	: 114.23 g/mol Source: HSDB
Solubility	: Water: 0.7 mg/l
Partition coefficient n-octanol/water (Log Pow)	: 5.18 Source: HSDB
Auto-ignition temperature	: 206 °C Source: ECHA
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: 0.96 – 6.5 % (V) Upper explosion limit: 1 – 6.5 % Source: ICSC
Explosive properties	: No data available
Oxidizing properties	: No data available

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9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

Vapors may form explosive mixture with air.

10.2. Chemical stability

Stable if stored under recommended conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5. Incompatible materials

Strong acids, Strong oxidizing agents.

10.6. Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral) : Not classified

Acute toxicity (dermal) : Not classified

Acute toxicity (inhalation) : Not classified

N-OCTANE-D18 (D, 99%) (111-65-9)	
LD50 oral rat	> 5000 mg/kg Source: ECHA
LC50 Inhalation - Rat	118000 mg/m ³ 4 h
ATE US (vapors)	118 mg/l/4h
ATE US (dust, mist)	118 mg/l/4h

Skin corrosion/irritation : Causes skin irritation.

Serious eye damage/irritation : Not classified

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Reproductive toxicity : Not classified

STOT-single exposure : May cause drowsiness or dizziness.

STOT-repeated exposure : Not classified

Aspiration hazard : May be fatal if swallowed and enters airways.

Viscosity, kinematic : No data available

Potential Adverse human health effects and symptoms : Burning sensation. Cough. Wheezing. Laryngitis. Shortness of breath. Headache. Nausea. Vomiting. Central nervous system depression. Narcosis.

Symptoms/effects after inhalation : May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.

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Symptoms/effects after skin contact	: May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/effects after eye contact	: May cause eye irritation.
Symptoms/effects after ingestion	: Aspiration hazard if swallowed - can enter lungs and cause damage. May be harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

N-OCTANE-D18 (D, 99%) (111-65-9)	
LC50 - Fish [1]	0.885 mg/l
EC50 - Crustacea [1]	0.18 mg/l
ErC50 algae	5.8 mg/l <i>Pseudokirchneriella subcapitata</i> - 72 h

12.2. Persistence and degradability

N-OCTANE-D18 (D, 99%) (111-65-9)	
Persistence and degradability	Not available.

12.3. Bioaccumulative potential

N-OCTANE-D18 (D, 99%) (111-65-9)	
Partition coefficient n-octanol/water (Log Pow)	5.18 Source: HSDB
Bioaccumulative potential	Not available.

12.4. Mobility in soil

N-OCTANE-D18 (D, 99%) (111-65-9)	
Ecology - soil	Not available.

12.5. Other adverse effects

Other adverse effects	: An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Very toxic to aquatic life with long lasting effects.
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SECTION 13: Disposal considerations

13.1. Disposal methods

Regional legislation (waste)	: Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.
Product/Packaging disposal recommendations	: Dispose in a safe manner in accordance with local/national regulations.
Ecology - waste materials	: Dispose of as unused product.

SECTION 14: Transport information

In accordance with DOT / TDG / IMDG / IATA

14.1. UN number

DOT NA No	: UN1262
UN-No. (TDG)	: UN1262
UN-No. (IMDG)	: 1262

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UN-No. (IATA) : 1262

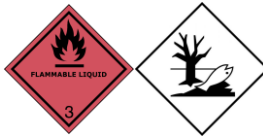
14.2. UN proper shipping name

Proper Shipping Name (DOT) : Octanes
Proper Shipping Name (TDG) : OCTANES
Proper Shipping Name (IMDG) : OCTANES
Proper Shipping Name (IATA) : Octanes

14.3. Transport hazard class(es)

DOT

Transport hazard class(es) (DOT) : 3
Hazard labels (DOT) : 3



TDG

Transport hazard class(es) (TDG) : 3
Hazard labels (TDG) : 3



IMDG

Transport hazard class(es) (IMDG) : 3
Hazard labels (IMDG) : 3



IATA

Transport hazard class(es) (IATA) : 3
Hazard labels (IATA) : 3



14.4. Packing group

Packing group (DOT) : II
Packing group (TDG) : II
Packing group (IMDG) : II
Packing group (IATA) : II

14.5. Environmental hazards

Dangerous for the environment : Yes

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Marine pollutant : Yes



Other information : No supplementary information available.

14.6. Special precautions for user

DOT

UN-No.(DOT) : UN1262
DOT Special Provisions (49 CFR 172.102) : IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized.
T4 - 2.65 178.274(d)(2) Normal..... 178.275(d)(3)
TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: tr is the maximum mean bulk temperature during transport, tf is the temperature in degrees celsius of the liquid during filling, and a is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling (tf) and the maximum mean bulk temperature during transportation (tr) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: d15 and d50 are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.
DOT Packaging Exceptions (49 CFR 173.xxx) : 150
DOT Packaging Non Bulk (49 CFR 173.xxx) : 202
DOT Packaging Bulk (49 CFR 173.xxx) : 242
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 60 L
DOT Vessel Stowage Location : B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.

TDG

UN-No. (TDG) : UN1262
Explosive Limit and Limited Quantity Index : 1 L
Excepted quantities (TDG) : E2
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index : 5 L
Emergency Response Guide (ERG) Number : 128

IMDG

Limited quantities (IMDG) : 1 L
Excepted quantities (IMDG) : E2
Packing instructions (IMDG) : P001
IBC packing instructions (IMDG) : IBC02
Tank instructions (IMDG) : T4
Tank special provisions (IMDG) : TP2
EmS-No. (Fire) : F-E - FIRE SCHEDULE Echo - NON-WATER-REACTIVE FLAMMABLE LIQUIDS
EmS-No. (Spillage) : S-E - SPILLAGE SCHEDULE Echo - FLAMMABLE LIQUIDS, FLOATING ON WATER
Stowage category (IMDG) : B
Flash point (IMDG) : '
Properties and observations (IMDG) : Colourless liquids. Explosive limits: 1% to 6.5% ISOCTANE: flashpoint-12°C c.c. n-OCTANE: flashpoint 13°C c.c. Immiscible with water.
MFAG-No : 128

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IATA

PCA Excepted quantities (IATA)	: E2
PCA Limited quantities (IATA)	: Y341
PCA limited quantity max net quantity (IATA)	: 1L
PCA packing instructions (IATA)	: 353
PCA max net quantity (IATA)	: 5L
CAO packing instructions (IATA)	: 364
CAO max net quantity (IATA)	: 60L
ERG code (IATA)	: 3H

14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

N-OCTANE-D18 (D, 99%) (111-65-9)

SARA Section 311/312 Hazard Classes	Fire hazard Immediate (acute) health hazard
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Commercial status of components according to the United States Environmental Protection Agency's Toxic Substances Control Act (TSCA):

Name	CAS-No.	Listing	Commercial status	Flags
N-OCTANE-D18 (D, 99%)	111-65-9	Present	Active	

15.2. International regulations

CANADA

N-OCTANE-D18 (D, 99%) (111-65-9)

Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

N-OCTANE-D18 (D, 99%) (111-65-9)

Listed on INSQ (Mexican National Inventory of Chemical Substances)
Listed on TECI (Thailand Existing Chemicals Inventory)

15.3. US State regulations

N-OCTANE-D18 (D, 99%) (111-65-9)

State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List
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SECTION 16: Other information

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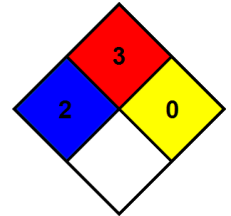
Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of H-phrases	
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
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

NFPA health hazard : 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard : 3 - Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 3 Serious Hazard - Materials capable of ignition under almost all normal temperature conditions. Includes flammable liquids with flash points below 73 F and boiling points above 100 F. as well as liquids with flash points between 73 F and 100 F. (Classes IB IC)

Physical : 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Safety Data Sheet (SDS), USA

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.