

Chemical Safety Data Sheet MSDS / SDS

N-OCTANE

Revision Date:2026-05-31 Revision Number:1

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

Product identifier

Product name : N-OCTANE
CBnumber : CB2124951
CAS : 111-65-9
EINECS Number : 203-892-1
Synonyms : octane,n-Octane

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P233 Keep container tightly closed.

P273 Avoid release to the environment.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P331 Do NOT induce vomiting.

Hazard statements

H225 Highly Flammable liquid and vapour

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

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|----------------------------------|
| Product name | : N-OCTANE |
| Synonyms | : octane,n-Octane |
| CAS | : 111-65-9 |
| EC number | : 203-892-1 |
| MF | : C ₈ H ₁₈ |
| MW | : 114.23 |

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

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

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.

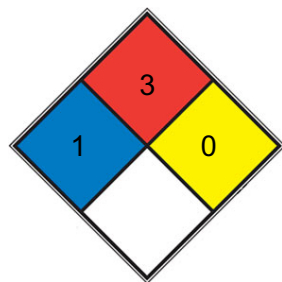
Forms explosive mixtures with air at ambient temperatures.

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.

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

NFPA 704



HEALTH 1 Exposure would cause irritation with only minor residual injury (e.g. [acetone](#), sodium bromate, potassium chloride)

Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature

FIRE 3 conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

SPEC.

HAZ.

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

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/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

Storage class (TRGS 510): 3: Flammable liquids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

| | |
|--|---|
| ['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis'] | ['n-octane', '111-65-9', 'PC-TWA', '500 mg/m ³ ', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.'] |
|--|---|

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

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 30 min

Material tested: KCL 741 L

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

Information on basic physicochemical properties

| | |
|---|---|
| a) Physical state | liquid |
| b) Color | colorless |
| c) Odor | characteristic |
| d) Melting point/freezing point | Melting point/range: -57 °C - lit. |
| e) Initial boiling point and boiling range | 125 - 127 °C - lit. |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 6.5 %(V) Lower explosion limit: 0.96 %(V) |
| h) Flash point | 13 °C - closed cup |
| i) Autoignition temperature | 220 °C |
| j) Decomposition temperature | No data available |
| k) pH | No data available |

| | |
|--|--|
| l) Viscosity | Viscosity, kinematic: 0.8 mm ² /s at 20 °C Viscosity, dynamic: No data available |
| m) Water solubility | ca.0.007 g/l at 20 °C |
| n) Partition coefficient n-octanol/water | log Pow: 5.15 |
| o) Vapor pressure | 14.7 hPa at 20.0 °C |
| p) Density | 0.703 g/cm ³ at 25 °C - lit. |
| Relative density | 0.703 g/mL at 25 °C(lit.) |
| q) Relative vapor density | 3.9 (vs air) |
| r) Particle characteristics | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |
| Solubility | ethanol: soluble(lit.) |
| Henry's Law Constant | 4.45 at 25 °C (Jnsson et al., 1982) |
| Dielectric constant | 1.1 (-4°C) |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.2 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents various plastics

10.3 Conditions to avoid

Warming.

10.4 Incompatible materials

No data available

10.5 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: The value is given in analogy to the following substances: isooctane

LC50 Inhalation - Rat - male and female - 4 h - > 24.88 mg/l - vapor (OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg (OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: isooctane

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: isooctane

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Remarks: 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: isooctane

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: The value is given in analogy to the following substances: n-heptane

Chromosome aberration test in vitro

Test system: rat hepatocytes

Method: OECD Test Guideline 473

Result: negative

Remarks: The value is given in analogy to the following substances: n-heptane

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: The value is given in analogy to the following substances: isooctane

No data available

Reproductive toxicity

Classified based on available data. For more details, see section 2

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

Classified based on available data. For more details, see section 2

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 LC50 - *Oryzias latipes* - 0.42 mg/l - 96.0 h

Remarks: (Lit.)

Toxicity to daphnia static test EC50 - *Daphnia magna* (Water flea) - 0.38 mg/l - 48 h and other aquatic Remarks: (ECOTOX Database) invertebrates

Toxicity to algae NOEC - *Pseudokirchneriella subcapitata* (microalgae) - 5.8 mg/l - 72 h

Remarks: (Lit.)

Toxicity to daphnia static test NOEC - *Daphnia magna* (Water flea) - 0.17 mg/l - 21 d and other aquatic (OECD Test Guideline 211) invertebrates(Chronic Remarks: (in analogy to similar products) toxicity)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 10 d

Result: 70.3 % - Readily biodegradable.

Remarks: (ECHA)

Theoretical oxygen 3,500 mg/g demand 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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1262

IMDG: 1262

IATA-DGR: 1262

14.2 UN proper shipping name

ADR/RID: OCTANES

IMDG: OCTANES

IATA-DGR: Octanes

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA-DGR: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.