

Chemical Safety Data Sheet MSDS / SDS

Octane SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: Octane
CAS: 111-65-9

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.in
Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090
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SECTION 2: Hazards identification**Classification of the substance or mixture**

Flammable liquids, Category 2
Skin irritation, Category 2

Aspiration hazard, Category 1
Specific target organ toxicity - single exposure, Category 3
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H315 Causes skin irritation
H304 May be fatal if swallowed and enters airways
H336 May cause drowsiness or dizziness
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P331 Do NOT induce vomiting.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P319 Get medical help if you feel unwell.
P391 Collect spillage.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Octane
Common names and synonyms:	Octane
CAS number:	111-65-9
EC number:	203-892-1
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Do NOT induce vomiting. Give nothing to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Inhalation of concentrated vapor may cause irritation of respiratory tract, depression, and pulmonary edema. Liquid can cause irritation of eyes and (on prolonged contact) irritation and cracking of skin. Ingestion causes irritation of mouth and stomach. Aspiration causes severe lung irritation, rapidly developing pulmonary edema, and central nervous system excitement, followed by depression. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aliphatic hydrocarbons and related compounds

SECTION 5: Firefighting measures**Suitable extinguishing media**

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

Specific hazards arising from the chemical

Behavior in Fire: Vapor is heavier than air and may travel a considerable distance to a source of ignition and flash back. (USCG, 1999)

Special protective actions for fire-fighters

Use powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. Personal protection: self-contained breathing apparatus.

Environmental precautions

Evacuate danger area! Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. Personal protection: self-contained breathing apparatus.

Methods and materials for containment and cleaning up

Evacuate danger area! Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Do NOT let this chemical enter the environment. Personal protection: self-contained breathing apparatus.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Prevent build-up of electrostatic charges (e.g., by grounding). Do NOT use compressed air for filling, discharging, or handling. Use non-sparking handtools. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong oxidants. Cool. Ventilation along the floor. Store in cool place. Keep container tightly closed in a

dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 300 ppm as TWA.MAK: 2400 mg/m³, 500 ppm; peak limitation category: II(2); pregnancy risk group: D

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state: Liquid. Liquid.

Colour: Colorless liquid

Odour:	Gasoline-like
Melting point/freezing point:	-56.8 °C
Boiling point or initial boiling point and boiling range:	124 - 126.6 °C. Atm. press.:1 atm. Remarks:Distillation range.
Flammability:	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 1.0% by volume; Upper flammable limit: 6.5% by volume.
Flash point:	13 °C.
Auto-ignition temperature:	206 °C.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	kinematic viscosity (in mm ² /s) = 0.801. Temperature:20°C.
Solubility:	Insoluble in water
Partition coefficient n-octanol/water:	log Pow = 5.15.
Vapour pressure:	1.86 kPa. Temperature:25 °C.
Density and/or relative density:	0.71 g/cm ³ . Temperature:15 °C.
Relative vapour density:	3.9 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

1000 ppm (IDLH based on 10% of the lower explosion limit for safety considerations even though the relevant toxicological data indicated that irreversible health effects or impairment of escape existed only at higher concentrations.)

Reacts with strong oxidants. This generates fire and explosion hazard. Attacks some forms of plastic, rubber and coatings.

Chemical stability

no data available

Possibility of hazardous reactions

A very dangerous fire hazard and severe explosion hazard when exposed to heat, flame, or oxidizers. The vapour is heavier than air and may travel along the ground; distant ignition possible. As a result of flow, agitation, etc., electrostatic charges can be generated. May be incompatible with strong oxidizing agents like nitric acid. Charring may occur followed by ignition of unreacted material and other nearby combustibles. In other settings, mostly unreactive. Not affected by aqueous solutions of acids, alkalis, most oxidizing agents, and most reducing agents. When heated sufficiently or when ignited in the presence of air, oxygen or strong oxidizing agents, burns exothermically to produce mostly carbon dioxide and water.

Conditions to avoid

no data available

Incompatible materials

Strong oxidizers.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - > 5 000 mg/kg bw.

Inhalation: LC50 - rat (male/female) - > 24.88 mg/L air (nominal).

Dermal: LD50 - rabbit (male/female) - > 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis. Exposure to high concentrations of vapour could cause lowering of consciousness.

STOT-repeated exposure

Repeated or prolonged contact with skin may cause dermatitis. The substance defats the skin, which may cause dryness or cracking.

Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LL50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 2.587 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 0.3 mg/L - 48 h.

Toxicity to algae: EL50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 2.084 mg/L - 72 h.

Toxicity to microorganisms: EL50 - *Tetrahymena pyriformis* - 10.86 mg/L - 48 h.

Persistence and degradability

The degradation of n-alkanes by microorganisms is similar to the degradation of fatty acids. The terminal methyl group is enzymatically oxidized by incorporation of molecular oxygen by a monooxygenase producing a primary alcohol with further oxidation to an acid group, although involvement of a dioxygenase is also postulated. Once the fatty acid is produced, it is degraded into 2-carbon units via the beta oxidation pathway. ... Another pathway for n-alkane degradation that is encountered less often is the oxidation of both terminal carbons to form a dioic acid with subsequent beta oxidation. Subterminal oxidation of the 2-carbon atom is seen mainly in C3-C6 alkanes, although it does occur in longer chain alkanes also. ... A dehydrogenation of the n-alkane may also occur yielding an alkene which is then converted to an alcohol, although there is little evidence for this theory. Some microorganisms have been shown to have both terminal and subterminal oxidation, each having very different rates of activity. The different chain lengths of n-alkanes are degraded to different extents ... At chain lengths greater than C6 the degradability generally increases until about C11-C12. /In a study comparing/ ... growth on long and short chain alkanes by some bacteria ... the initial oxygenase had a broad specificity and would oxidize C1-C8 alkanes ... /but/ cells grown on C4-C8 alkanes did not oxidize the shorter chain alkanes to a significant extent. ... n-Alkanes

Bioaccumulative potential

An estimated BCF of 1200 was calculated in fish for n-octane(SRC), using a log Kow of 5.18(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is very high(SRC).

Mobility in soil

The Koc of n-octane is estimated as 3.1×10^4 (SRC), using a log Kow of 5.18(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that n-octane is expected to be immobile in soil. Freundlich absorption coefficients of log 4.04 and log 3.49 were measured in Oberlausitz lignite (11.1% moisture content; 53.5 wt% carbon content; 0.6 wt % nitrogen content) and Pahokee peat soil (10.2% moisture content; 46.1 wt% carbon content; 3.3 wt % nitrogen content), respectively(4). Gaseous transport of volatile n-octane in unsaturated porous media was shown to be influenced by air-water interfacial adsorption and water-partitioning(5). Sorption of n-octane from air to snow was measured, resulting in a sorption coefficient of log -4.41 cu m/sq m at -6.8 deg C(6).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1262 (For reference only, please check.)

IMDG: UN1262 (For reference only, please check.)

IATA: UN1262 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: OCTANES (For reference only, please check.)

IMDG: OCTANES (For reference only, please check.)

IATA: OCTANES (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)

IMDG: 3 (For reference only, please check.)

IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: II (For reference only, please check.)

IMDG: II (For reference only, please check.)

IATA: II (For reference only, please check.)

Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

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

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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