SAFETY DATA SHEET according to the OSHA Hazard Communication Standard

Version 6.15
Revision Date 05/29/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Octane

Product Number : 74820
Brand : Sigma-Aldrich
Index-No. : 601-009-00-8
CAS-No. : 111-65-9

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids	:	Category 2
Skin irritation	:	Category 2
Specific target organ toxicity - single exposure	:	Category 3 (Central nervous system)
Aspiration hazard	:	Category 1
Short-term (acute) aquatic hazard	:	Category 1
Long-term (chronic) aquatic hazard	:	Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms :

Signal word : Danger

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.

Precautionary statements :

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.
P261 Avoid breathing mist or vapours.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

P301 + P310 IF SWALLOWED: Immediately call a

POISON CENTER/ doctor.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P331 Do NOT induce vomiting.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391 Collect spillage.

Storage:

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.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 111-65-9

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
n-octane	111-65-9*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.
TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this 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.
Most important symptoms and effects, both acute and delayed	:	The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Protection of first-aiders	:	For personal protection see section 8.
Notes to physician	:	No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	:	Carbon dioxide (CO2) Foam Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Pay attention to flashback. Vapours 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.
Hazardous combustion products	:	Carbon oxides
Specific extinguishing methods	:	No data available

Further information	:	Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Do not breathe vapours, 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. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter drains. Risk of explosion.
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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	:	Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	:	Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Further information on storage conditions	:	Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class : 3, Flammable liquids

Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
n-octane	111-65-9	TWA	75 ppm 350 mg/m3	NIOSH REL
		C	385 ppm 1,800 mg/m3	NIOSH REL
		TWA	500 ppm 2,350 mg/m3	OSHA Z-1
		TWA	300 ppm	ACGIH

Engineering measures : No data available

Personal protective equipment

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.

Recommended Filter type: : Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection
- Material : Nitrile rubber
- Break through time : 480 min
- Glove thickness : 0.4 mm
- Protective index : Full contact
- Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

- Material : Nitrile rubber
- Break through time : 30 min

Glove thickness	:	0.11 mm
Protective index	:	Splash contact
Manufacturer	:	KCL 741 Dermatril® L
Remarks	:	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).
Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	:	Flame retardant antistatic protective clothing.
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	liquid (68 °F / 20 °C, 1,013 hPa)
Color	:	colourless
Odor	:	characteristic
Odor Threshold	:	No data available
pH	:	No data available
Melting point/ range	:	-71 °F / -57 °C Method: lit.
Boiling point/boiling range	:	257 - 261 °F / 125 - 127 °C Method: lit.
Flash point	:	55 °F / 13 °C Method: closed cup
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available

Flammability (liquids)	:	No data available
Burning rate	:	No data available
Self-ignition	:	428 °F / 220 °C
Upper explosion limit / Upper flammability limit	:	Upper flammability limit 6.5 %(V)
Lower explosion limit / Lower flammability limit	:	Lower flammability limit 0.96 %(V)
Vapor pressure	:	14.7 hPa (68.0 °F / 20.0 °C)
Relative vapour density	:	No data available
Relative density	:	No data available
Density	:	0.70 g/cm3 (68 °F / 20 °C)
Solubility(ies)		
Water solubility	:	ca. 0.007 g/l (68 °F / 20 °C)
Partition coefficient: n-octanol/water	:	log Pow: 5.15
Autoignition temperature	:	428 °F / 220 °C
Decomposition temperature	:	No data available
Viscosity		
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	0.8 mm2/s (68 °F / 20 °C)
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Molecular weight	:	114.23 g/mol
Particle characteristics		
Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	Vapours may form explosive mixture with air.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	Violent reactions possible with: Strong oxidizing agents various plastics
Conditions to avoid	:	Warming.
Incompatible materials	:	No data available
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 - vapour

(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
Maximisation 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-heptaneTest Type: 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-heptaneTest Type: 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**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available

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
No data available

Aspiration hazard
Aspiration may cause pulmonary oedema 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

Ecotoxicity

Components:

n-octane:

Toxicity to fish	:	LC50 (Oryzias latipes): 0.42 mg/l End point: mortality Exposure time: 96.0 h Remarks: (Lit.)
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 0.38 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Remarks: (ECOTOX Database)
Toxicity to algae/aquatic plants	:	NOEC (Pseudokirchneriella subcapitata (microalgae)): 5.8 mg/l End point: Growth inhibition Exposure time: 72 h Remarks: (Lit.)
M-Factor (Acute aquatic toxicity)	:	1
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	:	NOEC (Daphnia magna (Water flea)): 0.17 mg/l Exposure time: 21 d Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 211 GLP: yes Remarks: (in analogy to similar products)

Ecotoxicology Assessment

Acute aquatic toxicity	:	Very toxic to aquatic life.
Chronic aquatic toxicity	:	Very toxic to aquatic life with long lasting effects.

Persistence and degradability

Components:

n-octane:

Biodegradability	:	aerobic Concentration: 3.3 mg/l Result: Readily biodegradable. Biodegradation: 70.3 % Exposure time: 10 d Remarks: (ECHA)
ThOD	:	3,500 mg/g Remarks: (Lit.)

Bioaccumulative potential

Components:

n-octane:

Partition coefficient: n-octanol/water	:	log Pow: 5.15

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential	:	Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues	:	Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other

waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No.	:	UN 1262
Proper shipping name	:	Octanes
Class	:	3
Packing group	:	II
Labels	:	Class 3 - Flammable liquids
Packing instruction (cargo aircraft)	:	364
Packing instruction (passenger aircraft)	:	353

IMDG-Code

UN number	:	UN 1262
Proper shipping name	:	OCTANES
Class	:	3
Packing group	:	II
Labels	:	3
EmS Code	:	F-E, S-E
Marine pollutant	:	yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number	:	UN 1262
Proper shipping name	:	Octanes
Class	:	3
Packing group	:	II
Labels	:	Class 3 - Flammable liquids
ERG Code	:	128
Marine pollutant	:	yes
Poison Inhalation Hazard	:	No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards	:	Fire Hazard Acute Health Hazard
SARA 313	:	This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).
This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.
This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.
This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307
This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

n-octane	111-65-9

Pennsylvania Right To Know

n-octane	111-65-9

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

US TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	:	USA. NIOSH Recommended Exposure Limits
OSHA Z-1	:	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
ACGIH / TWA	:	8-hour, time-weighted average
NIOSH REL / TWA	:	Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
NIOSH REL / C	:	Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA	:	8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA -

Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Revision Date : 05/29/2026

US / EN