SAFETY DATA SHEET

Version 8.12
Revision Date 29.05.2026
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Section 1: Identification

1.1 Product identifiers

Product name : n-Octane for synthesis

Product Number : 8.06910
Catalogue No. : 806910
Brand : Millipore
CAS-No. : 111-65-9

1.2 Other means of identification

No data available

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

Identified uses : Chemical for synthesis

1.4 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Pte Ltd
(Co. Registration No. 199403788W)
2 Science Park Drive
#05-01/12 Ascent Building
SINGAPORE 118222
SINGAPORE

Telephone : +65 6890 6633
Fax : +65 6890 6639
E-mail address : TechnicalService@merckgroup.com

1.5 Emergency telephone number

Emergency Phone # : +65 3158 1349 (CHEMTREC intl.) 800 101 2201 (CHEMTREC)

Section 2: Hazard identification

Classification of the substance or mixture

Flammable liquids : Category 2

Skin corrosion/irritation : Category 2

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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

GHS Label elements, including precautionary statements

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.
P261 Avoid breathing mist or vapours.
P264 Wash skin thoroughly after handling.
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.
P331 Do NOT induce vomiting.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391 Collect spillage.

Other hazards which do not result in classification

None known.

Section 3: Composition/information on ingredients

Substance / Mixture : Substance

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CAS-No. : 111-65-9

Components

Chemical name	CAS-No.	Concentration (% w/w)
n-octane	111-65-9	>= 90 -<= 100

Section 4: First-aid measures

Description of necessary 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

Risks : 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.

Indication of any immediate medical attention and special treatment needed

Treatment : No data available

Section 5: Fire-fighting measures

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.

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Special hazards arising from the substance or mixture

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

Special protective actions for fire-fighters

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

Section 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal precautions	:	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

Environmental precau-	:	Do not let product enter drains.

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tions		Risk of explosion.

Methods and materials for containment and cleaning up

Methods for 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.

Precautions for safe handling

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.
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Conditions for safe storage, including any incompatibilities

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.
Further information on storage stability	:	Store below +30°C.

Section 8: Exposure controls/personal protection

Control parameters

Occupational Exposure Limits

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis

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n-octane	111-65-9	PEL (long term)	300 ppm 1,400 mg/m3	SG OEL
		PEL (short term)	375 ppm 1,750 mg/m3	SG OEL
		TWA	300 ppm	ACGIH

Appropriate engineering control measures : No data available

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

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 : 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.

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-

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36124 Eichenzell, Internet: www.kcl.de).

Section 9: Physical and chemical properties

Appearance	:	liquid (20 °C , 1,013 hPa)
Color	:	colourless
Odor	:	characteristic
Odor Threshold	:	No data available
pH	:	No data available
Melting point/ range	:	-57 °C
Boiling point/boiling range	:	125 - 126 °C (1,013 hPa)
Flash point	:	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	:	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 (20.0 °C)
Relative vapour density	:	No data available
Relative density	:	No data available
Density	:	0.70 g/cm3 (20 °C)
Solubility(ies)		

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Water solubility	:	ca. 0.007 g/l (20 °C)
Partition coefficient: n-octanol/water	:	log Pow: 5.15
Autoignition temperature	:	220 °C
Decomposition temperature	:	No data available
Viscosity Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	0.8 mm2/s (20 °C)
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Molecular weight	:	114.26 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

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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: isooc-tane**Carcinogenicity**
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause drowsiness or dizziness. - Central nervous system

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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

Toxicity

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	:	EC50 (Daphnia magna (Water flea)): 0.38 mg/l

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other aquatic invertebrates		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

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Mobility in soil

No data available

Other adverse effects

No data available

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
UN proper shipping name	:	Octanes
Transport hazard class(es)	:	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
UN proper shipping name	:	OCTANES
Transport hazard class(es)	:	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.

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.

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Section 15: Regulatory information

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

Workplace Safety and Health Act and Workplace Safety and Health (General Provisions) Regulations: This product is subject to the requirements in the Act/Regulations.

Environmental Protection and Management Act and Environmental Protection and Management (Hazardous Substances) Regulations	:	Not applicable
Singapore Explosive Precursors (Guns, Explosives and Weapons Control Act, Second Schedule)	:	Not applicable
Fire Safety (Petroleum and Flammable Materials) Regulations	:	Octanes

Section 16: Other information

Revision Date	:	29.05.2026

Further information

Other information	:	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. Copyright 2025 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
Date format	:	dd.mm.yyyy

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
SG OEL	:	Singapore. Workplace Safety and Health Act - First Schedule Permissible Exposure Limits of Toxic Substances
ACGIH / TWA	:	8-hour, time-weighted average

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SG OEL / PEL (long term) : Permissible Exposure Level (PEL) Long Term
SG OEL / PEL (short term) : Permissible Exposure Level (PEL) Short Term

AIIC - Australian Inventory of Industrial Chemicals; ANTT - National Agency for Transport by Land of Brazil; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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; 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; MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods; n.o.s. - Not Otherwise Specified; Nch - Chilean Norm; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NOM - Official Mexican Norm; 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TDG - Transportation of Dangerous Goods; 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; WHMIS - Workplace Hazardous Materials Information System

SG / EN

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