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	:	Merck Life Science Pty Ltd Ground Floor, Building 1, 885 Mountain Highway BAYSWATER VIC 3153 AUSTRALIA
Telephone	:	+61 1800 800 097
E-mail address	:	customersupport.anz@merckgroup.com

1.5 Emergency telephone number

Emergency Phone #	:	Free call (24/7): 1800 862 115 Int'l (24/7): +61 2 9037 2994 (CHEMTREC)

SECTION 2. HAZARDS IDENTIFICATION

GHS Classification

Flammable liquids	:	Category 2
Skin corrosion/irritation	:	Category 2
Specific target organ toxicity - single exposure	:	Category 3 (Central nervous system)

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Aspiration hazard	:	Category 1
Short-term (acute) aquatic hazard	:	Category 1
Long-term (chronic) aquatic hazard	:	Category 1

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.
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.

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P362 + P364 Take off contaminated clothing and wash it before reuse.
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.

Other hazards which do not result in classification

None known.

SECTION **3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

CAS-No. : 111-65-9

Components

Chemical name	CAS-No.	Concentration (% w/w)
n-octane	111-65-9	>= 60 -<= 100

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 : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in

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acute and delayed		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	:	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.
Hazchem Code	:	3YE

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

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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	300 ppm 1,400 mg/m3	AU OEL
		STEL	375 ppm 1,750 mg/m3	AU OEL
		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

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		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.

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)

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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) 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

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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

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Method: OECD Test Guideline 476
Result: negative
Remarks: The value is given in analogy to the following substances: isooctane**Carcinogenicity**
No data available

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.

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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 inverte-brates	:	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 inverte-brates (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

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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

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
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

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Packing group	:	II
Labels	:	3
EmS Code	:	F-E, S-E
Marine pollutant	:	yes

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

Not applicable for product as supplied.

National Regulations

ADG

UN number	:	UN 1262
Proper shipping name	:	OCTANES
Class	:	3
Packing group	:	II
Labels	:	3
Hazchem Code	:	3YE
Environmentally hazardous	:	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**

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

Therapeutic Goods (Poisons Standard) Instrument	:	No poison schedule number allocated (Please use the original publication to check for specific uses, specific conditions or threshold limits that might apply for this chemical)
Prohibition/Licensing Requirements	:	There is no applicable prohibition, authorisation and restricted use requirements, including for carcinogens referred to in Schedule 10 of the model WHS Act and Regulations.
National Code of Practice for Chemicals of Security Concern	:	Not listed

Standard for the Uniform Scheduling of Medicines and Poisons - Poisons Schedule Number:

SECTION 16: ANY OTHER RELEVANT INFORMATION

Further information

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Revision Date	:	29.05.2026
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)
AU OEL	:	Australia. Workplace Exposure Standards for Airborne Contaminants.
ACGIH / TWA	:	8-hour, time-weighted average
AU OEL / TWA	:	Exposure standard - time weighted average
AU OEL / STEL	:	Exposure standard - short term exposure limit

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 Chem-

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icals; 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

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