



## SAFETY DATA SHEET

### n-octane

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

##### 1.1. Product identifier

Product name	n-octane
Product number	89967151
CAS number	111-65-9
EU index number	601-009-00-8
EC number	203-892-1

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

Identified uses	Research and development. Industrial use
Uses advised against	Not suitable for human consumption or veterinary purposes.

##### 1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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##### 1.4. Emergency telephone number

+44 (0) 7769276927

#### SECTION 2: Hazards identification

##### 2.1. Classification of the substance or mixture

###### Classification (SI 2019 No. 720)

Physical hazards	Flam. Liq. 2 - H225
Health hazards	Skin Irrit. 2 - H315 STOT SE 3 - H336 Asp. Tox. 1 - H304
Environmental hazards	Aquatic Acute 1 - H400 Aquatic Chronic 1 - H410

##### 2.2. Label elements

EC number	203-892-1
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###### Hazard pictograms



Signal word

Danger

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<b>Hazard statements</b>	H225 Highly flammable liquid and vapour. H315 Causes skin irritation. H336 May cause drowsiness or dizziness. H304 May be fatal if swallowed and enters airways. H410 Very toxic to aquatic life with long lasting effects.
<b>Precautionary statements</b>	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P240 Ground and bond container and receiving equipment. P241 Use explosion-proof electrical equipment. P242 Use non-sparking tools. P243 Take action to prevent static discharges. P261 Avoid breathing vapour/ spray. P264 Wash contaminated 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. P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. P302+P352 IF ON SKIN: Wash with plenty of water. P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P312 Call a POISON CENTRE/doctor if you feel unwell. P331 Do NOT induce vomiting. P332+P313 If skin irritation occurs: Get medical advice/ attention. P362+P364 Take off contaminated clothing and wash it before reuse. P391 Collect spillage. 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. P501 Dispose of contents/ container in accordance with national regulations.

### 2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

<b>Product name</b>	n-octane
<b>EU index number</b>	601-009-00-8
<b>CAS number</b>	111-65-9
<b>EC number</b>	203-892-1
<b>Chemical formula</b>	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> CH <sub>3</sub>

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

<b>General information</b>	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
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<b>Inhalation</b>	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention. Place unconscious person on their side in the recovery position and ensure breathing can take place.
<b>Ingestion</b>	Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on their side in the recovery position and ensure breathing can take place. Keep affected person under observation. Get medical attention if symptoms are severe or persist. Do not induce vomiting. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention immediately.
<b>Skin contact</b>	Rinse with water.
<b>Eye contact</b>	Remove any contact lenses and open eyelids wide apart. Rinse with water. Get medical attention if any discomfort continues.
<b>Protection of first aiders</b>	First aid personnel should wear appropriate protective equipment during any rescue.

### **4.2. Most important symptoms and effects, both acute and delayed**

<b>General information</b>	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
<b>Inhalation</b>	A single exposure may cause the following adverse effects: Headache. Nausea, vomiting. Central nervous system depression. Drowsiness, dizziness, disorientation, vertigo. Narcotic effect.
<b>Ingestion</b>	May cause irritation. Aspiration hazard if swallowed. Entry into the lungs following ingestion or vomiting may cause chemical pneumonitis.
<b>Skin contact</b>	Redness. Irritating to skin.
<b>Eye contact</b>	May be slightly irritating to eyes.

### **4.3. Indication of any immediate medical attention and special treatment needed**

<b>Notes for the doctor</b>	Treat symptomatically.
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## **SECTION 5: Firefighting measures**

### **5.1. Extinguishing media**

<b>Suitable extinguishing media</b>	The product is flammable. Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
<b>Unsuitable extinguishing media</b>	Do not use water jet as an extinguisher, as this will spread the fire.

### **5.2. Special hazards arising from the substance or mixture**

<b>Specific hazards</b>	Containers can burst violently or explode when heated, due to excessive pressure build-up. Flammable liquid and vapour. Vapours may be ignited by a spark, a hot surface or an ember. Vapours may form explosive mixtures with air. Fire-water run-off in sewers may create fire or explosion hazard.
<b>Hazardous combustion products</b>	Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours.

### **5.3. Advice for firefighters**

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<b>Protective actions during firefighting</b>	Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Ventilate closed spaces before entering them. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. If a leak or spill has not ignited, use water spray to disperse vapours and protect men stopping the leak. Avoid discharge to the aquatic environment. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.
<b>Special protective equipment for firefighters</b>	Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

### SECTION 6: Accidental release measures

#### 6.1. Personal precautions, protective equipment and emergency procedures

<b>Personal precautions</b>	Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Evacuate area. Provide adequate ventilation. No smoking, sparks, flames or other sources of ignition near spillage. Promptly remove any clothing that becomes contaminated. Avoid inhalation of vapours and spray/mists. Use suitable respiratory protection if ventilation is inadequate.
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#### 6.2. Environmental precautions

<b>Environmental precautions</b>	Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.
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#### 6.3. Methods and material for containment and cleaning up

<b>Methods for cleaning up</b>	Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Eliminate all ignition sources if safe to do so. No smoking, sparks, flames or other sources of ignition near spillage. Do not allow material to enter confined spaces, due to the risk of explosion. Absorb small quantities with paper towels and evaporate in a safe place. Once evaporation is complete, place paper in a suitable waste disposal container and seal securely. Large Spillages: If the product is soluble in water, dilute the spillage with water and mop it up. Alternatively, or if it is not water-soluble, absorb the spillage with an inert, dry material and place it in a suitable waste disposal container. The contaminated absorbent may pose the same hazard as the spilled material. Label the containers containing waste and contaminated materials and remove from the area as soon as possible. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dangerous for the environment. Do not empty into drains. For waste disposal, see Section 13.
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#### 6.4. Reference to other sections

<b>Reference to other sections</b>	For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.
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### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

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### Usage precautions

Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Handle all packages and containers carefully to minimise spills. Keep container tightly sealed when not in use. Avoid the formation of mists. The product is flammable. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Avoid discharge to the aquatic environment. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

### Advice on general occupational hygiene

Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

### 7.2. Conditions for safe storage, including any incompatibilities

#### Storage precautions

Store away from incompatible materials (see Section 10). Store locked up. Keep away from oxidising materials, heat and flames. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

#### Storage class

Flammable liquid storage.

### 7.3. Specific end use(s)

#### Specific end use(s)

The identified uses for this product are detailed in Section 1.2.

## SECTION 8: Exposure controls/Personal protection

### 8.1. Control parameters

### 8.2. Exposure controls

#### Protective equipment



#### Appropriate engineering controls

Provide adequate general and local exhaust ventilation. Ensure the ventilation system is regularly maintained and tested. Good general ventilation should be adequate to control worker exposure to airborne contaminants. Observe any occupational exposure limits for the product or ingredients.

#### Eye/face protection

Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses.

#### Hand protection

Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacturer, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, wear gloves that are proven to be impervious to the chemical and resist degradation. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.

#### Other skin and body protection

Wear appropriate clothing to prevent repeated or prolonged skin contact.

#### Hygiene measures

Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.

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<b>Respiratory protection</b>	Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.
<b>Environmental exposure controls</b>	Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

<b>Appearance</b>	Clear liquid.
<b>Colour</b>	Colourless.
<b>Odour</b>	Characteristic.
<b>Odour threshold</b>	No information available.
<b>pH</b>	No information available.
<b>Melting point</b>	-57°C/-70.6°F
<b>Initial boiling point and range</b>	No information available.
<b>Flash point</b>	13°C/55.4°F Closed cup.
<b>Evaporation rate</b>	No information available.
<b>Flammability (solid, gas)</b>	No information available.
<b>Upper/lower flammability or explosive limits</b>	No information available.
<b>Vapour pressure</b>	No information available.
<b>Vapour density</b>	No information available.
<b>Relative density</b>	0.703
<b>Solubility(ies)</b>	No information available.
<b>Partition coefficient</b>	No information available.
<b>Auto-ignition temperature</b>	220°C/428°F
<b>Decomposition Temperature</b>	No information available.

#### 9.2. Other information

<b>Refractive index</b>	1.3980
<b>Molecular weight</b>	114.23

### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

<b>Reactivity</b>	Forms explosive mixtures with air on intense heating.
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#### 10.2. Chemical stability

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**Stability** Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.

### 10.3. Possibility of hazardous reactions

**Possibility of hazardous reactions** The following materials may react strongly with the product: Oxidising agents.

### 10.4. Conditions to avoid

**Conditions to avoid** Avoid heat, flames and other sources of ignition. Containers can burst violently or explode when heated, due to excessive pressure build-up. Static electricity and formation of sparks must be prevented.

### 10.5. Incompatible materials

**Materials to avoid** Oxidising materials. Acids - oxidising.

### 10.6. Hazardous decomposition products

**Hazardous decomposition products** Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

#### Acute toxicity - oral

**Summary** Based on available data the classification criteria are not met.

#### Acute toxicity - dermal

**Summary** Based on available data the classification criteria are not met.

#### Acute toxicity - inhalation

**Summary** Based on available data the classification criteria are not met.

#### Skin corrosion/irritation

**Summary** Causes skin irritation.

#### Serious eye damage/irritation

**Summary** Based on available data the classification criteria are not met.

#### Respiratory sensitisation

**Summary** Based on available data the classification criteria are not met.

#### Skin sensitisation

**Summary** Based on available data the classification criteria are not met.

#### Germ cell mutagenicity

**Summary** Based on available data the classification criteria are not met.

#### Carcinogenicity

**Summary** Based on available data the classification criteria are not met.

#### IARC carcinogenicity

None of the ingredients are listed or exempt.

#### Reproductive toxicity

**Summary** Based on available data the classification criteria are not met.

#### Specific target organ toxicity - single exposure

**Summary** May cause drowsiness or dizziness.

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**Target organs** Central nervous system

### Specific target organ toxicity - repeated exposure

**Summary** Based on available data the classification criteria are not met.

### Aspiration hazard

**Summary** May be fatal if swallowed and enters airways. Pneumonia may be the result if vomited material containing solvents reaches the lungs.

**General information** The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

**Inhalation** A single exposure may cause the following adverse effects: Headache. Nausea, vomiting. Central nervous system depression. Drowsiness, dizziness, disorientation, vertigo. Narcotic effect.

**Ingestion** May cause irritation. Aspiration hazard if swallowed. Entry into the lungs following ingestion or vomiting may cause chemical pneumonitis.

**Skin contact** Redness. Irritating to skin.

**Eye contact** May be slightly irritating to eyes.

**Route of exposure** Ingestion Inhalation Skin and/or eye contact

**Target organs** Central nervous system

## SECTION 12: Ecological information

### 12.1. Toxicity

#### Acute aquatic toxicity

**Summary** Very toxic to aquatic life.

#### Chronic aquatic toxicity

**Summary** Very toxic to aquatic life with long lasting effects.

### 12.2. Persistence and degradability

**Persistence and degradability** The degradability of the product is not known.

### 12.3. Bioaccumulative potential

**Bioaccumulative potential** No data available on bioaccumulation.

**Partition coefficient** No information available.

### 12.4. Mobility in soil

**Mobility** No data available.

### 12.5. Results of PBT and vPvB assessment

### 12.6. Other adverse effects

**Other adverse effects** None known.

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods



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<b>General information</b>	The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.
<b>Disposal methods</b>	Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

### SECTION 14: Transport information

<b>General</b>	For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.
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#### 14.1. UN number

UN No. (ADR/RID)	1262
UN No. (IMDG)	1262
UN No. (ICAO)	1262
UN No. (ADN)	1262

#### 14.2. UN proper shipping name

Proper shipping name (ADR/RID)	OCTANES
Proper shipping name (IMDG)	OCTANES (n-Octane)
Proper shipping name (ICAO)	OCTANES
Proper shipping name (ADN)	OCTANES

#### 14.3. Transport hazard class(es)

ADR/RID class	3
ADR/RID classification code	F1
ADR/RID label	3
IMDG class	3
ICAO class/division	3
ADN class	3

#### Transport labels



#### 14.4. Packing group

ADR/RID packing group	II
IMDG packing group	II
ICAO packing group	II

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ADN packing group II

### 14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant



### 14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

EmS F-E, S-E

ADR transport category 2

Emergency Action Code 3YE

Hazard Identification Number 33  
(ADR/RID)

Tunnel restriction code (D/E)

### 14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Not applicable.

Annex II of MARPOL 73/78  
and the IBC Code

## SECTION 15: Regulatory information

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

National regulations Health and Safety at Work etc. Act 1974 (as amended).  
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].  
EH40/2005 Workplace exposure limits.

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

### Inventories

#### EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

## SECTION 16: Other information

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<b>Abbreviations and acronyms used in the safety data sheet</b>	<p>ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.</p> <p>ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.</p> <p>RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.</p> <p>IATA: International Air Transport Association.</p> <p>ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.</p> <p>IMDG: International Maritime Dangerous Goods.</p> <p>CAS: Chemical Abstracts Service.</p> <p>ATE: Acute Toxicity Estimate.</p> <p>LC50: Lethal Concentration to 50 % of a test population.</p> <p>LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).</p> <p>EC<sub>50</sub>: 50% of maximal Effective Concentration.</p> <p>PBT: Persistent, Bioaccumulative and Toxic substance.</p> <p>vPvB: Very Persistent and Very Bioaccumulative.</p>
<b>Classification abbreviations and acronyms</b>	<p>Flam. Liq. = Flammable liquid</p> <p>Asp. Tox. = Aspiration hazard</p> <p>Skin Irrit. = Skin irritation</p> <p>STOT SE = Specific target organ toxicity-single exposure</p> <p>Aquatic Acute = Hazardous to the aquatic environment (acute)</p> <p>Aquatic Chronic = Hazardous to the aquatic environment (chronic)</p>
<b>Classification procedures according to SI 2019 No. 720</b>	<p>Asp. Tox. 1 - H304: STOT SE 3 - H336: Skin Irrit. 2 - H315: : Expert judgement. Aquatic Acute 1 - H400: Aquatic Chronic 1 - H410: : Expert judgement. Flam. Liq. 2 - H225: : Expert judgement.</p>
<b>Training advice</b>	Only trained personnel should use this material.
<b>Revision date</b>	07/06/2022
<b>Revision</b>	1
<b>SDS number</b>	981
<b>Hazard statements in full</b>	<p>H225 Highly flammable liquid and vapour.</p> <p>H304 May be fatal if swallowed and enters airways.</p> <p>H315 Causes skin irritation.</p> <p>H336 May cause drowsiness or dizziness.</p> <p>H400 Very toxic to aquatic life.</p> <p>H410 Very toxic to aquatic life with long lasting effects.</p>

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.