# SAFETY DATA SHEET

Version 5.2 Revision Date 07/03/2014 Print Date 09/09/2014

## 1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Octane

Product Number : 296988
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, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich

3050 Spruce Street SAINT LOUIS MO 63103

USA

Telephone : +1 800-325-5832 Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

# 2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

## GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 2), H225 Skin irritation (Category 2), H315

Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

Aspiration hazard (Category 1), H304 Acute aquatic toxicity (Category 1), H400 Chronic aquatic toxicity (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word Danger

Hazard statement(s)

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 statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P233 Keep container tightly closed.

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P240 Ground/bond container and receiving equipment. P241 Use explosion-proof electrical/ventilating/lighting/equipment. P242 Use only non-sparking tools. Take precautionary measures against static discharge. P243 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray. P261 Wash skin thoroughly after handling. P264 Use only outdoors or in a well-ventilated area. P271 Avoid release to the environment. P273 Wear protective gloves/ protective clothing/ eye protection/ face P280 protection. P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician. P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower. IF INHALED: Remove victim to fresh air and keep at rest in a position P304 + P340 comfortable for breathing. P312 Call a POISON CENTER or doctor/physician if you feel unwell. Specific treatment (see supplemental first aid instructions on this label). P321 P331 Do NOT induce vomiting. If skin irritation occurs: Get medical advice/ attention. P332 + P313 Take off contaminated clothing and wash before reuse. P362 P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction. P391 Collect spillage. Store in a well-ventilated place. Keep container tightly closed. P403 + P233 Store in a well-ventilated place. Keep cool. P403 + P235 P405 Store locked up. P501 Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

# 3. COMPOSITION/INFORMATION ON INGREDIENTS

# 3.1 Substances

Synonyms : n-Octane

Formula : C<sub>8</sub>H<sub>18</sub>

Molecular Weight : 114.23 g/mol
CAS-No. : 111-65-9
EC-No. : 203-892-1
Index-No. : 601-009-00-8

**Hazardous components** 

Component	Classification	Concentration	
Octane			
	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H304, H315, H336, H410		

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

# 4.1 Description of first aid measures

## **General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

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#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

## In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

## 4.2 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

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

no data available

## 5. FIREFIGHTING MEASURES

## 5.1 Extinguishing media

# Suitable extinguishing media

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

## 5.2 Special hazards arising from the substance or mixture

Carbon oxides

## 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

## 5.4 Further information

Use water spray to cool unopened containers.

## 6. ACCIDENTAL RELEASE MEASURES

## 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

## 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

# 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

## 6.4 Reference to other sections

For disposal see section 13.

## 7. HANDLING AND STORAGE

## 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

## 7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

hygroscopic

## 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

## 8.1 Control parameters

Components with workplace control parameters

	an workplace co.			la :
Component	CAS-No.	Value	Control	Basis
			parameters	
Octane	111-65-9	TWA	300 ppm	USA. ACGIH Threshold Limit Values
				(TLV)
	Remarks	Upper Respiratory Tract irritation		
		TWA	75 ppm	USA. NIOSH Recommended
			350 mg/m3	Exposure Limits
		С	385 ppm	USA. NIOSH Recommended
			1,800 mg/m3	Exposure Limits
		15 minute ceiling value		
		TWA	500 ppm	USA. Occupational Exposure Limits
			2,350 mg/m3	(OSHA) - Table Z-1 Limits for Air
				Contaminants
		The value	in mg/m3 is approx	kimate.
		TWA	300 ppm	USA. OSHA - TABLE Z-1 Limits for
			1,450 mg/m3	Air Contaminants - 1910.1000
		STEL	375 ppm	USA. OSHA - TABLE Z-1 Limits for
			1,800 mg/m3	Air Contaminants - 1910.1000

## 8.2 Exposure controls

## Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

## Personal protective equipment

## Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm Break through time: 480 min

Material tested: Dermatril® P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

## **Body Protection**

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

# **Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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# Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

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

**Appearance** Form: liquid

Colour: colourless

characteristic b) Odour Odour Threshold no data available d) рΗ no data available

Melting point/freezing e)

point

Melting point/range: -57 °C (-71 °F) - lit.

Initial boiling point and f)

boiling range

125 - 127 °C (257 - 261 °F) - lit.

g) Flash point 13.0 °C (55.4 °F) - closed cup

h) Evapouration rate no data available Flammability (solid, gas) no data available

Upper/lower flammability or explosive limits Upper explosion limit: 6.5 %(V) Lower explosion limit: 0.96 %(V)

14.7 hPa (11.0 mmHg) at 20.0 °C (68.0 °F) Vapour pressure

Vapour density no data available

m) Relative density 0.703 g/cm3 at 25 °C (77 °F) n) Water solubility ca.0.007 g/l at 20 °C (68 °F)

Partition coefficient: n-

octanol/water

log Pow: 5.15

Auto-ignition temperature

220.0 °C (428.0 °F)

Decomposition

no data available

temperature

Viscosity no data available r) Explosive properties no data available Oxidizing properties no data available

#### 9.2 Other safety information

no data available

## 10. STABILITY AND REACTIVITY

#### 10.1 Reactivity

no data available

# 10.2 Chemical stability

Stable under recommended storage conditions.

#### Possibility of hazardous reactions 10.3

Vapours may form explosive mixture with air.

## 10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

#### 10.5 Incompatible materials

Strong acids, Strong oxidizing agents

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## 10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

# 11. TOXICOLOGICAL INFORMATION

## 11.1 Information on toxicological effects

## **Acute toxicity**

LC50 Inhalation - rat - 4 h - 118,000 mg/m3

Dermal: no data available

no data available

## Skin corrosion/irritation

no data available

## Serious eye damage/eye irritation

no data available

## Respiratory or skin sensitisation

no data available

## Germ cell mutagenicity

no data available

## 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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a

carcinogen or potential carcinogen by ACGIH.

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 identified as a

carcinogen or potential carcinogen by OSHA.

## Reproductive toxicity

no data available

no data available

## Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

# Specific target organ toxicity - repeated exposure

no data available

## **Aspiration hazard**

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

# **Additional Information**

RTECS: RG8400000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Central nervous system depression, narcosis

## 12. ECOLOGICAL INFORMATION

## 12.1 Toxicity

Toxicity to fish mortality LC50 - Oryzias latipes - 0.42 mg/l - 96.0 h

Toxicity to daphnia and Immobilization EC50 - Daphnia magna (Water flea) - 0.38 mg/l - 48 h

other aquatic invertebrates

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Toxicity to algae Growth inhibition NOEC - Pseudokirchneriella subcapitata - 5.8 mg/l - 72 h

# 12.2 Persistence and degradability

no data available

## 12.3 Bioaccumulative potential

no data available

# 12.4 Mobility in soil

no data available

## 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Very toxic to aquatic life.

## 13. DISPOSAL CONSIDERATIONS

## 13.1 Waste treatment methods

## **Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

## Contaminated packaging

Dispose of as unused product.

## 14. TRANSPORT INFORMATION

DOT (US)

UN number: 1262 Class: 3 Packing group: II

Proper shipping name: Octanes

Marine pollutant: No

Poison Inhalation Hazard: No

**IMDG** 

UN number: 1262 Class: 3 Packing group: II EMS-No: F-E, S-E

Proper shipping name: OCTANES

Marine pollutant: No

IATA

UN number: 1262 Class: 3 Packing group: II

Proper shipping name: Octanes

# 15. REGULATORY INFORMATION

# **SARA 302 Components**

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

## **SARA 313 Components**

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.

## SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

## **Massachusetts Right To Know Components**

 CAS-No.
 Revision Date

 Octane
 111-65-9
 1993-04-24

**Pennsylvania Right To Know Components** 

 CAS-No.
 Revision Date

 Octane
 111-65-9
 1993-04-24

# **New Jersey Right To Know Components**

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 CAS-No.
 Revision Date

 Octane
 111-65-9
 1993-04-24

## California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

# 16. OTHER INFORMATION

## Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute Acute aquatic toxicity
Aquatic Chronic Chronic aquatic toxicity
Asp. Tox. Aspiration hazard
Flam. Lig. Flammable liquids

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.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.

Skin Irrit. Skin irritation

**HMIS Rating** 

Health hazard: 0
Chronic Health Hazard:
Flammability: 3
Physical Hazard 0

**NFPA Rating** 

Health hazard: 2
Fire Hazard: 3
Reactivity Hazard: 0

## **Further information**

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# **Preparation Information**

Sigma-Aldrich Corporation Product Safety – Americas Region 1-800-521-8956

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