SAFETY DATA SHEET

Creation Date 04-Feb-2010 **Revision Date** 19-Dec-2025 **Revision Number** 6

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name **n-Octane**

Cat No. : **AC396900000; AC396900010; AC396901000**

CAS No 111-65-9
Synonyms No information available

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company
Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number
For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No. **US:**001-800-424-9300 / **Europe:**001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 2
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Central nervous system (CNS).	
Aspiration Toxicity	Category 1

Label Elements

Signal Word
Danger

Hazard Statements
Highly flammable liquid and vapor
May be fatal if swallowed and enters airways
Causes skin irritation
Causes serious eye irritation
May cause drowsiness or dizziness

Precautionary Statements
Prevention
Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
Keep container tightly closed
Ground and bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Keep cool
Take action to prevent static discharges
Use non-sparking tools
Inhalation
IF INHALED: Remove person to fresh air and keep comfortable for breathing
Call a POISON CENTER or doctor if you feel unwell
Skin
If skin irritation occurs: Get medical advice/attention
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
Take off contaminated clothing and wash before reuse
Eyes
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention
Ingestion
IF SWALLOWED: Immediately call a POISON CENTER or doctor
Do NOT induce vomiting
Fire
In case of fire: Use CO2, dry chemical, or foam to extinguish
Storage
Store locked up
Store in a well-ventilated place. Keep container tightly closed
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)
Very toxic to aquatic life with long lasting effects

Hazards classified under paragraph (d)(1)(ii) of 1910.1200
No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %

Octane	111-65-9	>95

4. First-aid measures

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Get medical attention.

Inhalation Remove to fresh air. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required. If not breathing, give artificial respiration. Risk of serious damage to the lungs (by aspiration).

Ingestion Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.

Most important symptoms and effects Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

Unsuitable Extinguishing Media No information available

Flash Point 13 °C / 55.4 °F

Method - No information available

Autoignition Temperature 220 °C / 428 °F

Explosion Limits

Upper 6.5 vol %

Lower 0.8 vol %

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Do not allow run-off from fire-fighting to enter drains or water courses.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO_2).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health	Flammability	Instability	Physical hazards
3	3	0	N/A

6. Accidental release measures

Personal Precautions Evacuate personnel to safe areas. Remove all sources of ignition. Use personal protective equipment as required. Ensure adequate ventilation. Take precautionary measures against static discharges.

Environmental Precautions Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

Methods for Containment and Clean Up Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges. Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

7. Handling and Storage

Handling Wear personal protective equipment/face protection. Ensure adequate ventilation. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.

Storage. Flammables area. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Octane	TWA: 300 ppm	(Vacated) TWA: 300 ppm (Vacated) TWA: 1450 mg/m³ (Vacated) STEL: 375 ppm (Vacated) STEL: 1800 mg/m³ TWA: 500 ppm TWA: 2350 mg/m³	IDLH: 1000 ppm REL = 75 ppm (TWA) REL = 350 mg/m³ (TWA) Ceiling: 385 ppm Ceiling: 1800 mg/m³	TWA: 300 ppm TWA: 1450 mg/m³

Legend

ACGIH - American Conference of Governmental Industrial Hygienists
OSHA - Occupational Safety and Health Administration
NIOSH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended Filter type: Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State	Liquid		
Color	Colorless		
Odor	Petroleum distillates		
Odor Threshold	No information available		
Property	**Values**	**Remarks**	**• Method**
Melting Point/Range	-57 °C / -70.6 °F		
Softening Point	No data available		
Boiling Point/Range	125 - 127 °C / 257 - 260.6 °F	@ 760 mmHg	
Flash Point	13 °C / 55.4 °F	**Method -** No information available	
Flammability (liquid)	Highly flammable	On basis of test data	
Flammability (solid,gas)	Not applicable	Liquid	
Explosion Limits	**Lower** 0.8 Vol% **Upper** 6.5 Vol%		
Autoignition Temperature	220 °C / 428 °F		
Decomposition Temperature	No data available		
pH	Not applicable		
Viscosity	0.55 mPa.s at 20 °C		
Water Solubility	Insoluble	practically insoluble	
Solubility in other solvents	No information available		

Partition Coefficient (n-octanol/water)

Component	**log Pow**
Octane	5.18

Vapor Pressure	14 mbar @ 20 °C	
Density / Specific Gravity	0.708	
Bulk Density	Not applicable	Liquid
Vapor Density	3.9	(Air = 1.0)
Particle characteristics	(liquid) Not applicable	

Other Information

Molecular Formula	C8 H18
Molecular Weight	114.23
Explosive Properties	Vapors may form explosive mixtures with air
Evaporation Rate	0.6 (Butyl Acetate = 1.0)

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition. Temperatures above 200°C.

Incompatible Materials Strong oxidizing agents

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO_2)

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation May cause irritation of respiratory tract. May be harmful if inhaled. INHALATION MAY CAUSE CENTRAL NERVOUS SYSTEM EFFECTS.

Ingestion May be harmful if swallowed. Aspiration hazard. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhea. Harmful if swallowed. Potential for aspiration if swallowed.

Eyes Irritating to eyes.

Skin Irritating to skin. May be harmful in contact with skin.

Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Octane	>5 g/kg (Rat)	>2 g/kg (Rabbit)	LC50 > 24.88 mg/L (Rat) 4 h

Toxicologically Synergistic Products No information available

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available

Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity;

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Octane	111-65-9	Not listed	Not listed	Not listed	Not listed	Not listed

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Central nervous system (CNS).

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Category 1

Symptoms / effects,both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

Other Adverse Effects The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following

substances which are hazardous for the environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Octane	Not listed	Not listed	EC50 = 890 mg/L 30 min	EC50: = 0.38 mg/L, 48h (water flea)

Persistence and Degradability May persist based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility. Is not likely mobile in the environment due its low water solubility.

Component	log Pow
Octane	5.18

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No UN1262
Proper Shipping Name OCTANES
Hazard Class 3
Packing Group II

TDG

UN-No UN1262
Proper Shipping Name OCTANES
Hazard Class 3
Packing Group II

IATA

UN-No UN1262
Proper Shipping Name OCTANES
Hazard Class 3
Packing Group II

IMDG/IMO

UN-No UN1262
Proper Shipping Name OCTANES
Hazard Class 3
Packing Group II

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Octane	111-65-9	X	ACTIVE	-

Legend:
TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)
X - Listed
'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Octane	111-65-9	X	-	203-892-1	X	X	X	X	X	KE-26612

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Octane	X	X	X	-	X

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant Y
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade Serious risk, Grade 3

Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) -	REACH (1907/2006) -	REACH Regulation (EC

		Annex XIV - Substances Subject to Authorization	Annex XVII - Restrictions on Certain Dangerous Substances	1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Octane	111-65-9	-	Use restricted. See entry 75. (see link for restriction details)	-

REACH links
https://echa.europa.eu/substances-restricted-under-reach

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Octane	111-65-9	Listed	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?
Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Octane	111-65-9	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By
Product stewardship (Regulatory Affairs)
Thermo Fisher Scientific
email - begel.sdsdesk@thermofisher.com

Creation Date 04-Feb-2010
Revision Date 19-Dec-2025
Print Date 19-Dec-2025
Revision Summary Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The 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, unless specified in the text

End of SDS