

SAFETY DATA SHEET

Revision Date 19-Dec-2025

Revision Number 5

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 Octyl isocyanate

Cat No. : AC416460000; AC416460050; AC416460100

CAS No 3158-26-7
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 4
Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Respiratory Sensitization	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Danger

Hazard Statements

Combustible liquid
Causes skin irritation
Causes serious eye irritation
May cause allergy or asthma symptoms or breathing difficulties if inhaled
May cause respiratory irritation
Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
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
In case of inadequate ventilation wear respiratory protection
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
Keep cool

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing
If experiencing respiratory symptoms: Call a POISON CENTER or doctor

Skin

IF ON SKIN: Wash with plenty of soap and water
Call a POISON CENTER or doctor if you feel unwell
If skin irritation occurs: Get medical advice/attention
Take off contaminated clothing

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: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam to extinguish

Storage

Store in a well-ventilated place. Keep container tightly closed
Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
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Octane, 1-isocyanato-	3158-26-7	99
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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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.
Inhalation	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.
Ingestion	Clean mouth with water. Get medical attention.
Most important symptoms and effects	Difficulty in breathing. May cause allergy or asthma symptoms or breathing difficulties if inhaled. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Carbon dioxide (CO ₂). Foam. Dry chemical. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	71 °C / 159.8 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Combustible material. Flammable. Containers may explode when heated.

Hazardous Combustion Products

Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid).

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.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	See Section 12 for additional Ecological Information.

Methods for Containment and Clean Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder,

Up sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition.

7. Handling and Storage

Handling Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Handle product only in closed system or provide appropriate exhaust ventilation. Keep away from open flames, hot surfaces and sources of ignition.

Storage. Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents. Strong acids. Strong bases. Alcohols. Amines.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

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

Color

Odor

Odor Threshold

Property

Melting Point/Range

Softening Point

Boiling Point/Range

Flash Point

Flammability (liquid)

Flammability (solid,gas)

Explosion Limits

Liquid

Off-white

No information available

No information available

Values

No data available

No data available

200 - 204 °C / 392 - 399.2 °F

71 °C / 159.8 °F

Combustible liquid

Not applicable

No data available

Remarks

Method

@ 760 mmHg

Method - No information available

On basis of test data

Liquid

Autoignition Temperature

Decomposition Temperature

pH

Viscosity

No data available

No data available

No information available

No data available

Water Solubility	DECOMPOSES IN WATER	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

Other Information

Molecular Formula	C ₉ H ₁₇ N O
Molecular Weight	155.24
Explosive Properties	explosive air/vapour mixtures possible

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions. Moisture sensitive.
Conditions to Avoid	Heat, flames and sparks. Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents, Strong acids, Strong bases, Alcohols, Amines
Hazardous Decomposition Products	Nitrogen oxides (NO _x), Carbon monoxide (CO), Carbon dioxide (CO ₂), Hydrogen cyanide (hydrocyanic acid)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	Not an expected route of exposure.
Ingestion	May be harmful if swallowed.
Eyes	Avoid contact with eyes. Irritating to eyes. Lachrymator (substance which increases the flow of tears).
Skin	Avoid contact with skin. May cause irritation. Harmful in contact with skin.

Toxicology data for the components

Toxicologically Synergistic Products	No information available
(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization;	
Respiratory	Category 1
Skin	No data available
	No information 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, 1-isocyanato-	3158-26-7	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 Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

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

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

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

Do not empty into drains.

Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

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 UN2206
Hazard Class 6.1
Packing Group III

TDG

UN-No UN2206
Hazard Class 6.1

Packing Group	III
IATA	
UN-No	UN2206
Proper Shipping Name	ISOCYANATES, TOXIC, N.O.S.*
Hazard Class	6.1
Packing Group	III
IMDG/IMO	
UN-No	UN2206
Proper Shipping Name	Isocyanates, toxic, n.o.s.
Hazard Class	6.1
Packing Group	III

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Octane, 1-isocyanato-	3158-26-7	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, 1-isocyanato-	3158-26-7	-	X	221-598-1	-	-	X	-	-	-

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 Not applicable

U.S. Department of Transportation

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

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

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Octane, 1-isocyanato-	3158-26-7	-	-	-

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, 1-isocyanato-	3158-26-7	Not applicable	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, 1-isocyanato-	3158-26-7	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By Product stewardship (Regulatory Affairs)
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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