

SAFETY DATA SHEET

Creation Date 16-Sep-2010

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 1-Octyne

Cat No. : AC223510000; AC223510250; AC223511000

CAS No 629-05-0
Synonyms Hexylacetylene

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
Aspiration Toxicity

Category 2
Category 1

Label Elements

Signal Word
Danger

Hazard Statements

Highly flammable liquid and vapor
May be fatal if swallowed and enters airways

**Precautionary Statements****Prevention**

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
Wear protective gloves/protective clothing/eye protection/face protection
Take action to prevent static discharges
Use non-sparking tools

Skin

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

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 cool

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 %
1-Octyne	629-05-0	>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. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. 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. Get medical attention. 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	Difficulty in breathing. . Inhalation of high vapor concentrations may cause symptoms like

effects	headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	17 °C / 62.6 °F
Method -	No information available
Autoignition Temperature	225 °C / 437 °F
Explosion Limits	
Upper	No data available
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.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂).

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	Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Should not be released into the environment. See Section 12 for additional Ecological Information.
Methods for Containment and Clean Up	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and Storage

Handling	Ensure adequate ventilation. Wear personal protective equipment/face protection. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges. Wash hands before breaks and immediately after handling the product. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded.
Storage.	Keep containers tightly closed in a dry, cool and well-ventilated place. Flammables area. Keep away from heat, sparks and flame. Incompatible Materials. Strong oxidizing agents.

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	Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. Ensure adequate ventilation, especially in confined areas.
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	No protective equipment is needed under normal use conditions.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance			
Physical State	Liquid		
Color	Colorless, Yellow		
Odor	Characteristic		
Odor Threshold	No information available		
Property	Values	Remarks	• Method
Melting Point/Range	-80 °C / -112 °F		
Softening Point	No data available		
Boiling Point/Range	127 - 128 °C / 260.6 - 262.4 °F	@ 760 mmHg	
Flash Point	17 °C / 62.6 °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%		
Autoignition Temperature	225 °C / 437 °F		
Decomposition Temperature	No data available		
pH	No information available		
Viscosity	No data available		
Water Solubility	No information available		
Solubility in other solvents	No information available		
Partition Coefficient (n-octanol/water)			
Component	log Pow		
1-Octyne	3.50		
Vapor Pressure	18 hPa (25°C)		
Density / Specific Gravity	0.740		
Bulk Density	Not applicable	Liquid	
Vapor Density	3.8	(Air = 1.0)	
Particle characteristics	Not applicable (liquid)		
Other Information			
Molecular Formula	C8 H14		
Molecular Weight	110.2		
Explosive Properties	Vapors may form explosive mixtures with air		

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.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	May be harmful if inhaled. May cause irritation of respiratory tract.
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	May cause irritation.
Skin	May be harmful in contact with skin. May cause irritation.

Toxicology data for the components

Toxicologically Synergistic Products	No information available
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(b) skin corrosion/irritation;	No data available
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(c) serious eye damage/irritation;	No data available
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(d) respiratory or skin sensitization;	
Respiratory	No data available
Skin	No data available

(e) germ cell mutagenicity;	No data available
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(f) carcinogenicity;

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

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
1-Octyne	629-05-0	Not listed	Not listed	Not listed	Not listed	Not listed

(g) reproductive toxicity;	No data available
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(h) STOT-single exposure;	No data available
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(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	Category 1
Other Adverse Effects	The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information
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. See actual entry in RTECS for complete information.
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	Persistence is unlikely
Bioaccumulation/ Accumulation	No information available.
Mobility	.

Component	log Pow
1-Octyne	3.50

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.
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14. Transport information

DOT

UN-No	UN3295
Proper Shipping Name	Hydrocarbons, liquid, n.o.s.
Technical Shipping Name	(1-OCTYNE)
Hazard Class	3
Packing Group	II

TDG

UN-No	UN3295
Proper Shipping Name	Hydrocarbons, liquid, n.o.s.
Technical Shipping Name	(1-OCTYNE)
Hazard Class	3
Packing Group	II

IATA

UN-No	UN3295
Proper Shipping Name	Hydrocarbons, liquid, n.o.s.
Technical Shipping Name	(1-OCTYNE)
Hazard Class	3
Packing Group	II

IMDG/IMO

UN-No	UN3295
Proper Shipping Name	Hydrocarbons, liquid, n.o.s.
Technical Shipping Name	(1-OCTYNE)
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
1-Octyne	629-05-0	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
1-Octyne	629-05-0	-	X	211-069-3	X	-	X	X	-	KE-26781

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)
1-Octyne	629-05-0	-	-	-

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)
1-Octyne	629-05-0	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)
1-Octyne	629-05-0	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

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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