

SAFETY DATA SHEET

Creation Date 24-Nov-2009

Revision Date 13-Oct-2023

Revision Number 8

1. Identification

Product Name 0.1% Trifluoroacetic acid in Acetonitrile

Cat No. : LS121-1; LS121-4; LS121-212; LS121-500; HB9813-4;
HB9813RS200ASME; NC1647052; NC9811516; NC0395568

Synonyms 0.1% TFA in Acetonitrile (Optima LC/MS; HPLC)

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

Emergency Telephone Number

CHEMTREC®, Inside the USA: 800-424-9300
CHEMTREC®, Outside the USA: 001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Serious Eye Damage/Eye Irritation	Category 2

Label Elements

Signal Word

Danger

Hazard Statements

Highly flammable liquid and vapor
Harmful if swallowed, in contact with skin or if inhaled

Causes serious eye irritation



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
 Keep away from heat/sparks/open flames/hot surfaces. - No smoking
 Keep container tightly closed
 Ground/bond container and receiving equipment
 Use explosion-proof electrical/ventilating/lighting equipment
 Use only non-sparking tools
 Take precautionary measures against static discharge

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
 Call a POISON CENTER or doctor/physician if you feel unwell

Skin

Call a POISON CENTER or doctor/physician if you feel unwell
 Wash contaminated clothing before reuse
 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

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 for extinction

Storage

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

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Acetonitrile	75-05-8	99.9
Trifluoroacetic acid	76-05-1	0.1

4. First-aid measures

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.
 Immediate medical attention is required.

Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
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.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Most important symptoms and effects	Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Metabolism may release cyanide, which may result in headache, dizziness, weakness, collapse, unconsciousness, and possible death
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	Water may be ineffective, Do not use a solid water stream as it may scatter and spread fire
Flash Point	12.8 °C / 55.0 °F
Method -	Estimated
Autoignition Temperature	524 °C / 975.2 °F
Explosion Limits	
Upper	16.00 vol %
Lower	4.4 vol %
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Flammable. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated.

Hazardous Combustion Products

Hydrogen cyanide (hydrocyanic acid). Nitrogen oxides (NO_x). 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 2	Flammability 3	Instability 0	Physical hazards N/A
--------------------	--------------------------	-------------------------	--------------------------------

6. Accidental release measures

Personal Precautions	Remove all sources of ignition. Take precautionary measures against static discharges. Keep people away from and upwind of spill/leak. Ensure adequate ventilation. Use personal protective equipment as required. Do not get in eyes, on skin, or on clothing.
Environmental Precautions	Should not be released into the environment. See Section 12 for additional Ecological Information.
Methods for Containment and Clean Up	Remove all sources of ignition. Take precautionary measures against static discharges. Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling	Use only under a chemical fume hood. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Do not breathe mist/vapors/spray. Use only non-sparking tools. 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. Keep away from heat, sparks and flame. Flammables area. Incompatible Materials. Strong oxidizing agents. Strong acids. Reducing Agent.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
Acetonitrile	TWA: 20 ppm Skin	(Vacated) TWA: 40 ppm (Vacated) TWA: 70 mg/m ³ (Vacated) TWA: 5 mg/m ³ (Vacated) STEL: 60 ppm (Vacated) STEL: 105 mg/m ³ TWA: 40 ppm TWA: 70 mg/m ³	IDLH: 137 ppm IDLH: 25 mg/m ³ TWA: 20 ppm TWA: 34 mg/m ³	TWA: 20 ppm

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 adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. 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:	low boiling organic solvent. Type AX. Brown. conforming to EN371.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Clear
Odor	pungent
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-50 °C / -58 °F

Boiling Point/Range	82 °C / 179.6 °F @ 760 mmHg
Flash Point	12.8 °C / 55.0 °F
Method -	Estimated
Evaporation Rate	5.79 (Butyl Acetate = 1.0)
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	16.00 vol %
Lower	4.4 vol %
Vapor Pressure	No information available
Vapor Density	1.42 (Air = 1.0)
Specific Gravity	0.7810
Solubility	Miscible with water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	524 °C / 975.2 °F
Decomposition Temperature	No information available
Viscosity	No information available

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products. Heat, flames and sparks. Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents, Strong acids, Reducing Agent
Hazardous Decomposition Products	Hydrogen cyanide (hydrocyanic acid), Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Oral LD50

Category 4. ATE = 300 - 2000 mg/kg.

Dermal LD50

Category 4. ATE = 1000 - 2000 mg/kg.

Vapor LC50

Category 4. ATE = 10 - 20 mg/l.

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Acetonitrile	450-787 mg/kg (Rat) 2460 mg/kg (Rat)	> 2000 mg/kg (Rabbit)	LC50 = 3587 ppm (6.022 mg/l) (Mouse) 4h LC50 = 16,000 ppm (26.8 mg/l) (Rat) 4h
Trifluoroacetic acid	200-400 mg/kg (rat)	Not listed	10 mg/L/2h (rat)

Toxicologically Synergistic No information available

Products

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	Irritating to eyes
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico

Acetonitrile	75-05-8	Not listed	Not listed	Not listed	Not listed	Not listed
Trifluoroacetic acid	76-05-1	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting; Metabolism may release cyanide, which may result in headache, dizziness, weakness, collapse, unconsciousness, and possible death

Endocrine Disruptor Information No information available

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

12. Ecological information

Ecotoxicity

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants. Do not empty into drains.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Acetonitrile	Not listed	LC50: = 1850 mg/L, 96h static (Lepomis macrochirus) LC50: = 1000 mg/L, 96h static (Pimephales promelas) LC50: 1600 - 1690 mg/L, 96h flow-through (Pimephales promelas) LC50: = 1650 mg/L, 96h static (Poecilia reticulata)	EC50 = 28000 mg/L 48 h EC50 = 73 mg/L 24 h EC50 = 7500 mg/L 15 h	Not listed
Trifluoroacetic acid	Not listed	Zebrafish: LC50: >1000 mg/L/96h	Not listed	daphnia: EC50: 55 mg/L/24h

Persistence and Degradability Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

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

Component	log Pow
Acetonitrile	-0.34
Trifluoroacetic acid	-2.1

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.

Component	RCRA - U Series Wastes	RCRA - P Series Wastes
Acetonitrile - 75-05-8	U003	-

14. Transport information

DOT

UN-No UN1648
 Proper Shipping Name ACETONITRILE SOLUTION
 Hazard Class 3
 Packing Group II

TDG

UN-No UN1648
 Proper Shipping Name ACETONITRILE SOLUTION
 Hazard Class 3
 Packing Group II

IATA

UN-No UN1648
 Proper Shipping Name ACETONITRILE SOLUTION
 Hazard Class 3
 Packing Group II

IMDG/IMO

UN-No UN1648
 Proper Shipping Name ACETONITRILE SOLUTION
 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
Acetonitrile	75-05-8	X	ACTIVE	-
Trifluoroacetic acid	76-05-1	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
Acetonitrile	75-05-8	X	-	200-835-2	X	X	X	X	X	KE-00067
Trifluoroacetic acid	76-05-1	X	-	200-929-3	X	X	X	X	X	KE-34233 X

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

U.S. Federal Regulations**SARA 313**

Component	CAS No	Weight %	SARA 313 - Threshold Values %
Acetonitrile	75-05-8	99.9	1.0

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act)

Component	CWA - Hazardous Substances	CWA - Reportable Quantities	CWA - Toxic Pollutants	CWA - Priority Pollutants
Acetonitrile	-	-	X	X

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Acetonitrile	X		-

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA This material, as supplied, contains one or more substances regulated as a hazardous substance under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302)

Component	Hazardous Substances RQs	CERCLA EHS RQs
Acetonitrile	5000 lb	-

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
Acetonitrile	X	X	X	X	X
Trifluoroacetic acid	-	X	-	-	-

U.S. Department of Transportation

Reportable Quantity (RQ): Y
 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 No information available

Authorisation/Restrictions according to EU REACH

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)
Acetonitrile	75-05-8	-	Use restricted. See item 75. (see link for restriction details)	-
Trifluoroacetic acid	76-05-1	-	Use restricted. See item 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)
Acetonitrile	75-05-8	Listed	Not applicable	Not applicable	Not applicable
Trifluoroacetic acid	76-05-1	Listed	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin List)
Trifluoroacetic acid (CAS #: 76-05-1)	-	Listed	Listed	Listed	Listed

PFAS Legend

Listed = Meets the PFAS definition of the named authority

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)
Acetonitrile	75-05-8	Not applicable	Not applicable	Not applicable	Not applicable
Trifluoroacetic acid	76-05-1	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By

Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Creation Date

24-Nov-2009

Revision Date

13-Oct-2023

Print Date

13-Oct-2023

Revision Summary

This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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