

according to Regulation (EC) No. 1907/2006

Creation Date 09-Dec-2022 Revision Date 24-Mar-2024 Revision Number 2

# SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Cat No. : T85176

1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use Laboratory chemicals.

Sector of use SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites

**Product category** PC21 - Laboratory chemicals

**Process categories** PROC15 - Use as a laboratory reagent

Environmental release category ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)

Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company

Thermo Fisher (Kandel) GmbH

Erlenbachweg 2, 76870 Kandel, Germany

Tel: +49 (0) 721 84007 280 Fax: +49 (0) 721 84007 300

**Swiss distributor -** Fisher Scientific AG Neuhofstrasse 11, CH 4153 Reinach

Tel: +41 (0) 56 618 41 11

https://www.fishersci.ch/ch/en/customer-help-

support/forms/email-us.html

**E-mail address** begel.sdsdesk@thermofisher.com

1.4. 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

customers in Switzerland:

Tox Info Suisse Emergency Number: 145 (24hr)

Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)

Chemtrec (24h) Toll-Free: 0800 564 402 Chemtrec Local: +41-43 508 20 11 (Zurich)

# **SECTION 2: HAZARDS IDENTIFICATION**

#### 2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

#### Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Revision Date 24-Mar-2024

# **Physical hazards**

Flammable liquids Category 2 (H225)

#### **Health hazards**

Acute oral toxicity

Acute dermal toxicity

Acute Inhalation Toxicity - Vapors

Serious Eye Damage/Eye Irritation

Category 4 (H302)

Category 4 (H312)

Category 4 (H332)

Category 2 (H319)

#### **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

#### 2.2. Label elements



# Signal Word

#### **Danger**

# **Hazard Statements**

H225 - Highly flammable liquid and vapor

H319 - Causes serious eye irritation

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

#### **Precautionary Statements**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

P312 - Call a POISON CENTER or doctor if you feel unwell

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P280 - Wear protective gloves/protective clothing/eye protection/face protection

# 2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

Toxicity to Soil Dwelling Organisms

Toxic to terrestrial vertebrates

This product does not contain any known or suspected endocrine disruptors

# **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Revision Date 24-Mar-2024

#### 3.2. Mixtures

Component	CAS No	EC No	Weight %	CLP Classification - Regulation (EC) No 1272/2008
Acetonitrile	75-05-8	200-835-2	99.82	Flam. Liq. 2 (H225) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Eye Irrit. 2 (H319) Acute Tox. 4 (H332)
Trifluoroacetic acid	76-05-1	EEC No. 200-929-3	0.18	Skin Corr 1A (H314) Eye Dam. 1 (H318) Acute Tox. 4 (H332) Aquatic Chronic 3 (H412) EUH071

Component	ECHA (RAC) ATE (Oral)	ECHA (RAC) ATE (Dermal)	ECHA (RAC) ATE (Inhalation)	
Acetonitrile	ATE = 617  mg/kg	=	-	

ECHA (RAC) - Committee for Risk Assessment - European CHemicals Agency ATE - Acute Toxiciy Estimate; mg/kg bw - milligrams per kilogram of body weight

Full text of Hazard Statements: see section 16

# **SECTION 4: FIRST AID MEASURES**

#### 4.1. Description of first aid measures

**General Advice** If symptoms persist, call a physician.

**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. If skin irritation persists,

call a physician.

**Ingestion** Clean mouth with water and drink afterwards plenty of water.

Inhalation Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if

symptoms occur.

Self-Protection of the First Aider Ensure that medical personnel are aware of the material(s) involved, take precautions to

protect themselves and prevent spread of contamination.

4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable. . Inhalation of high vapor concentrations may cause

symptoms like headache, dizziness, tiredness, nausea and vomiting

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

Notes to Physician Treat symptomatically.

# **SECTION 5: FIREFIGHTING MEASURES**

#### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water mist may be used to cool closed containers.

\_\_\_\_\_

Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

# Extinguishing media which must not be used for safety reasons

No information available.

#### 5.2. Special hazards arising from the substance or mixture

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 oxides, Nitrogen oxides (NOx), Hydrogen fluoride.

# 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

# **SECTION 6: ACCIDENTAL RELEASE MEASURES**

#### 6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

#### 6.2. Environmental precautions

Should not be released into the environment.

#### 6.3. Methods and material for containment and cleaning 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.

#### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

# **SECTION 7: HANDLING AND STORAGE**

#### 7.1. Precautions for safe handling

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

# **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

#### 7.2. Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat, sparks and flame.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3 Storage Class (LGK) (Germany)

ALFAAT85176

Revision Date 24-Mar-2024

Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Revision Date 24-Mar-2024

Switzerland - Storage of hazardous substances

Storage class - SC 3

https://www.kvu.ch/de/themen/stoffe-und-produkte https://www.kvu.ch/fr/themes/substances-et-produits https://www.kvu.ch/it/temi/sostanze-e-prodotti

# 7.3. Specific end use(s)

Use in laboratories

# **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

#### 8.1. Control parameters

# **Exposure limits**

List source(s): **EU** - Commission Directive (EU) 2019/1831 of 24 October 2019 establishing a fifth list of indicative occupational exposure limit values pursuant to Council Directive 98/24/EC and amending Commission Directive 2000/39/EC **UK** - EH40/2005 Work Exposure Limits, Forth edition. Published 2020. **IRE** - 2010 Code of Practice for the Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001. Published by the Health and Safety Authority. **CH** - The Government of Switzerland has set a directive on limit values for working materials (Grenzwerte am Arbeitsplatz) which is based on the Swiss Federal Regulation "Verordnung über die Verhütung von Unfällen und Berufskrankheiten". This directive is administered, periodically revised and enforced by SUVA (Swiss National Accident Insurance Fund).

Component	European Union	The United Kingdom	France	Belgium	Spain
Acetonitrile	TWA: 40 ppm (8hr)	STEL: 60 ppm 15 min	TWA / VME: 40 ppm (8	TWA: 20 ppm 8 uren	TWA / VLA-ED: 40 ppm
	TWA: 70 mg/m <sup>3</sup> (8hr)	STEL: 102 mg/m <sup>3</sup> 15	heures). restrictive limit	TWA: 34 mg/m <sup>3</sup> 8 uren	(8 horas)
	Skin	min	TWA / VME: 70 mg/m <sup>3</sup>	Huid	TWA / VLA-ED: 68
		TWA: 40 ppm 8 hr	(8 heures). restrictive		mg/m³ (8 horas)
		TWA: 68 mg/m <sup>3</sup> 8 hr	limit TWA / VME: 5		Piel
		_	mg/m³ (8 heures).		
			Peau		

Component	Italy	Germany	Portugal	The Netherlands	Finland
Acetonitrile	TWA: 20 ppm 8 ore.	TWA: 10 ppm (8	TWA: 40 ppm 8 horas	TWA: 34 mg/m <sup>3</sup> 8 uren	TWA: 20 ppm 8 tunteina
	Time Weighted Average	Stunden). AGW -	TWA: 70 mg/m <sup>3</sup> 8 horas		TWA: 34 mg/m <sup>3</sup> 8
	TWA: 35 mg/m <sup>3</sup> 8 ore.	exposure factor 2	Pele		tunteina
	Time Weighted Average	TWA: 17 mg/m <sup>3</sup> (8			STEL: 40 ppm 15
	Pelle	Stunden). AGW -			minuutteina
		exposure factor 2			STEL: 68 mg/m <sup>3</sup> 15
		TWA: 10 ppm (8			minuutteina
		Stunden). MAK			lho
		TWA: 17 mg/m <sup>3</sup> (8			
		Stunden). MAK TWA: 2			
		mg/m³ (8 Stunden).			
		MAK			
		Höhepunkt: 20 ppm			
		Höhepunkt: 34 mg/m <sup>3</sup>			
		Höhepunkt: 2 mg/m <sup>3</sup>			
		Haut			

Component	Austria	Denmark	Switzerland	Poland	Norway
Acetonitrile	Haut	TWA: 40 ppm 8 timer	Haut/Peau	STEL: 140 mg/m <sup>3</sup> 15	TWA: 30 ppm 8 timer
	MAK-KZGW: 160 ppm	TWA: 70 mg/m <sup>3</sup> 8 timer	STEL: 40 ppm 15	minutach	TWA: 50 mg/m <sup>3</sup> 8 timer
	15 Minuten	STEL: 80 ppm 15	Minuten	TWA: 70 mg/m <sup>3</sup> 8	TWA: 5 mg/m <sup>3</sup> 8 timer
	MAK-KZGW: 280 mg/m <sup>3</sup>	minutter	STEL: 68 mg/m <sup>3</sup> 15	godzinach	STEL: 45 ppm 15
	15 Minuten	STEL: 140 mg/m <sup>3</sup> 15	Minuten	_	minutter. value
	MAK-TMW: 40 ppm 8	minutter	TWA: 20 ppm 8		calculated
	Stunden	Hud	Stunden		STEL: 75 mg/m <sup>3</sup> 15
	MAK-TMW: 70 mg/m <sup>3</sup> 8		TWA: 34 mg/m <sup>3</sup> 8		minutter. value
	Stunden		Stunden		calculated
					Hud

Component	Bulgaria	Croatia	Ireland	Cyprus	Czech Republic
Acetonitrile	TWA: 40 ppm	kože	TWA: 40 ppm 8 hr.	TWA: 40 ppm	TWA: 70 mg/m <sup>3</sup> 8
	TWA: 70 mg/m <sup>3</sup>	TWA-GVI: 40 ppm 8	TWA: 70 mg/m <sup>3</sup> 8 hr.	TWA: 70 mg/m <sup>3</sup>	hodinách.
	Skin notation	satima.	STEL: 120 ppm 15 min	_	Potential for cutaneous

#### Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Revision Date 24-Mar-2024

TWA-GVI: 70 mg/m <sup>3</sup> 8	STEL: 310 mg/m <sup>3</sup> 15	absorption
satima.	min	Ceiling: 100 mg/m <sup>3</sup>
	Skin	

Component	Estonia	Gibraltar	Greece	Hungary	Iceland
Acetonitrile	Nahk	Skin notation	STEL: 60 ppm	TWA: 70 mg/m <sup>3</sup> 8	TWA: 40 ppm 8
	TWA: 40 ppm 8	TWA: 40 ppm 8 hr	STEL: 105 mg/m <sup>3</sup>	órában. AK	klukkustundum.
	tundides.	TWA: 70 mg/m <sup>3</sup> 8 hr	TWA: 40 ppm	lehetséges borön	TWA: 70 mg/m <sup>3</sup> 8
	TWA: 70 mg/m <sup>3</sup> 8	_	TWA: 70 mg/m <sup>3</sup>	keresztüli felszívódás	klukkustundum.
	tundides.		_		Skin notation
					Ceiling: 80 ppm
					Ceiling: 140 mg/m <sup>3</sup>

Component	Latvia	Lithuania	Luxembourg	Malta	Romania
Acetonitrile	skin - potential for	TWA: 40 ppm IPRD		possibility of significant	Skin notation
	cutaneous exposure	TWA: 70 mg/m <sup>3</sup> IPRD	uptake through the skin	uptake through the skin	TWA: 40 ppm 8 ore
	TWA: 40 ppm	Oda	TWA: 40 ppm 8	TWA: 40 ppm	TWA: 70 mg/m <sup>3</sup> 8 ore
	TWA: 70 mg/m <sup>3</sup>		Stunden	TWA: 70 mg/m <sup>3</sup>	
			TWA: 70 mg/m <sup>3</sup> 8		
			Stunden		
Trifluoroacetic acid	TWA: 2 mg/m <sup>3</sup>	TWA: 2 mg/m³ IPRD			
	_	Oda			

Component	Russia	Slovak Republic	Slovenia	Sweden	Turkey
Acetonitrile	MAC: 10 mg/m <sup>3</sup>	Potential for cutaneous	TWA: 40 ppm 8 urah	Indicative STEL: 60 ppm	Deri
		absorption	TWA: 70 mg/m <sup>3</sup> 8 urah	15 minuter	TWA: 40 ppm 8 saat
		TWA: 40 ppm	Koža	Indicative STEL: 100	TWA: 70 mg/m <sup>3</sup> 8 saat
		TWA: 70 mg/m <sup>3</sup>	STEL: 140 mg/m <sup>3</sup> 15	mg/m <sup>3</sup> 15 minuter	
			minutah	TLV: 30 ppm 8 timmar.	
			STEL: 80 ppm 15	NGV	
			minutah	TLV: 50 mg/m <sup>3</sup> 8	
				timmar. NGV	
				Hud	
Trifluoroacetic acid	Skin notation				
	MAC: 2 mg/m <sup>3</sup>				

# **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

# Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

See table for values

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Acetonitrile 75-05-8 ( 99.82 )				DNEL = 32.2mg/kg bw/day

	Component	Acute effects local	Acute effects	Chronic effects local	Chronic effects
_					

#### Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

	(Inhalation)	systemic (Inhalation)	(Inhalation)	systemic (Inhalation)
Acetonitrile	DNEL = 40.6 ppm	DNEL = 40.6 ppm	DNEL = 40.6 ppm	DNEL = 40.6 ppm
75-05-8 ( 99.82 )	(68 mg/m <sup>3</sup> )	(68 mg/m <sup>3</sup> )	(68 mg/m <sup>3</sup> )	(68 mg/m <sup>3</sup> )
Trifluoroacetic acid	DNEL = 16mg/m <sup>3</sup>		$DNEL = 2.67 \text{mg/m}^3$	
76-05-1 ( 0.18 )				

#### **Predicted No Effect Concentration (PNEC)**

See values below.

Component	Fresh water	Fresh water	Water Intermittent	Microorganisms in	Soil (Agriculture)
		sediment		sewage treatment	
Acetonitrile	PNEC = 10mg/L	PNEC = 7.53 mg/kg	PNEC = 10mg/L	PNEC = 32mg/L	PNEC = 2.41 mg/kg
75-05-8 ( 99.82 )		sediment dw			soil dw
Trifluoroacetic acid	PNEC = 0.56mg/L	PNEC = 2.36mg/kg	PNEC = 2.37mg/L	PNEC = 83.2mg/L	PNEC = 4.7µg/kg
76-05-1 ( 0.18 )	-	sediment dw	_	-	soil dw

Component	Marine water	Marine water sediment	Marine water Intermittent	Food chain	Air
Acetonitrile 75-05-8 ( 99.82 )	PNEC = 1mg/L				
Trifluoroacetic acid 76-05-1 ( 0.18 )	PNEC = 0.056mg/L	PNEC = 0.236mg/kg sediment dw			

#### 8.2. Exposure controls

#### **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.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

**Eye Protection** Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material Nitrile rubber Neoprene Natural rubber	Breakthrough time See manufacturers recommendations	Glove thickness	<b>EU standard</b> EN 374	Glove comments (minimum requirement)
PVC				

Skin and body protection Long sleeved clothing.

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

Respiratory Protection When workers are facing concentrations above the exposure limit they must use

appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used

and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 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

ALFAAT85176

Revision Date 24-Mar-2024

Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure

limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN

Revision Date 24-Mar-2024

141

When RPE is used a face piece Fit Test should be conducted

**Environmental exposure controls** No information available.

# **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

# 9.1. Information on basic physical and chemical properties

Physical State Liquid

**Appearance** 

Odor No information available
Odor Threshold No data available
Melting Point/Range No data available
Softening Point No data available
Boiling Point/Range No information available

Flammability (liquid)Highly flammableEstimatedFlammability (solid,gas)Not applicableLiquid

Explosion Limits No data available

Flash Point No information available Method - No information available

Autoignition TemperatureNo data availableDecomposition TemperatureNo data availablepHNot applicableViscosityNo data availableWater SolubilityNo information availableSolubility in other solventsNo information available

Partition Coefficient (n-octanol/water)

Component log Pow
Acetonitrile -0.34
Trifluoroacetic acid -2.1

Vapor Pressure

Density / Specific Gravity

No data available
No data available

Bulk DensityNot applicableLiquidVapor DensityNo data available(Air = 1.0)

Particle characteristics Not applicable (liquid)

9.2. Other information

**Explosive Properties** Vapors may form explosive mixtures with air

# **SECTION 10: STABILITY AND REACTIVITY**

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous PolymerizationNo information available.Hazardous ReactionsNone under normal processing.

Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition.

Revision Date 24-Mar-2024

Page 9/14

10.5. Incompatible materials

None known.

#### 10.6. Hazardous decomposition products

Carbon oxides. Nitrogen oxides (NOx). Hydrogen fluoride.

# SECTION 11: TOXICOLOGICAL INFORMATION

#### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### **Product Information**

(a) acute toxicity;

Oral Category 4

Based on available data, the classification criteria are not met

**Dermal** Category 4

Based on available data, the classification criteria are not met

Inhalation Category 4

Based on available data, the classification criteria are not met

#### Toxicology data for the components

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Acetonitrile	450-787 mg/kg (Rat)	> 2000 mg/kg (Rabbit)	LC50 = 3587 ppm (6.022 mg/l)
	2460 mg/kg (Rat)		(Mouse) 4h
			LC50 = 16,000 ppm (26.8 mg/l)
			(Rat) 4h
Trifluoroacetic acid	200-400 mg/kg (rat)	-	10 mg/L/2h (rat)

Component	ECHA (RAC) ATE (Oral)	ECHA (RAC) ATE (Dermal)	ECHA (RAC) ATE (Inhalation)
Acetonitrile	ATE = 617 mg/kg	-	-

ECHA (RAC) - Committee for Risk Assessment - European CHemicals Agency ATE - Acute Toxiciy Estimate; mg/kg bw - milligrams per kilogram of body weight

(b) skin corrosion/irritation; Based on available data, the classification criteria are not met

(c) serious eye damage/irritation; Category 2 Based on available data, the classification criteria are not met

(d) respiratory or skin sensitization;

**Respiratory**Skin
Based on available data, the classification criteria are not met
Based on available data, the classification criteria are not met

(e) germ cell mutagenicity; Based on available data, the classification criteria are not met

(f) carcinogenicity; Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; Based on available data, the classification criteria are not met

(h) STOT-single exposure; Based on available data, the classification criteria are not met

Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

(i) STOT-repeated exposure; Based on available data, the classification criteria are not met

**Target Organs** None known.

(j) aspiration hazard; Based on available data, the classification criteria are not met

delayed

Symptoms / effects,both acute and Inhalation of high vapor concentrations may cause symptoms like headache, dizziness,

Revision Date 24-Mar-2024

tiredness, nausea and vomiting.

11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any

known or suspected endocrine disruptors.

# **SECTION 12: ECOLOGICAL INFORMATION**

12.1. Toxicity

**Ecotoxicity effects** 

Component	Freshwater Fish	Water Flea	Freshwater Algae
Acetonitrile	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)		
Trifluoroacetic acid	Zebrafish: LC50: >1000 mg/L/96h	daphnia: EC50: 55 mg/L/24h	_

Component	Microtox	M-Factor
Acetonitrile	EC50 = 28000 mg/L 48 h	
	EC50 = 73 mg/L 24 h	
	EC50 = 7500 mg/L 15 h	

12.2. Persistence and degradability No information available **Persistence** Persistence is unlikely.

12.3. Bioaccumulative potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Acetonitrile	-0.34	No data available
Trifluoroacetic acid	-2.1	No data available

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB

assessment

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent

and very bioaccumulative (vPvB).

12.6. Endocrine disrupting

properties

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

Revision Date 24-Mar-2024

12.7. Other adverse effects

Persistent Organic Pollutant Ozone Depletion Potential This product does not contain any known or suspected substance This product does not contain any known or suspected substance

# **SECTION 13: DISPOSAL CONSIDERATIONS**

13.1. Waste treatment methods

Waste from Residues/Unused

**Products** 

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging** 

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

**European Waste Catalogue (EWC)** 

According to the European Waste Catalog, Waste Codes are not product specific, but

application specific.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

Switzerland - Waste Ordinance

Disposal should be in accordance with applicable regional, national and local laws and regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance,

ADWO) SR 814.600

https://www.fedlex.admin.ch/eli/cc/2015/891/en

# **SECTION 14: TRANSPORT INFORMATION**

# IMDG/IMO

**14.1. UN number** UN1648

14.2. UN proper shipping name ACETONITRILE

14.3. Transport hazard class(es) 3
14.4. Packing group II

<u>ADR</u>

**14.1. UN number** UN1648

14.2. UN proper shipping name ACETONITRILE

14.3. Transport hazard class(es) 3 14.4. Packing group II

IATA

**14.1. UN number** UN1648

14.2. UN proper shipping name ACETONITRILE

14.3. Transport hazard class(es) 3 14.4. Packing group II

14.5. Environmental hazards No hazards identified

**14.6. Special precautions for user** No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments

Not applicable, packaged goods

# **SECTION 15: REGULATORY INFORMATION**

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

# **International Inventories**

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS), Taiwan (TCSI), Japan (ISHL), New Zealand (NZIoC), Japan (ISHL). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Acetonitrile	75-05-8	200-835-2	1	-	X	X	KE-00067	X	Х
Trifluoroacetic acid	76-05-1	200-929-3	-	-	Х	Х	KE-34233 X	Χ	Х

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Acetonitrile	75-05-8	X	ACTIVE	X	-	X	Х	X
Trifluoroacetic acid	76-05-1	Х	ACTIVE	X	-	Х	Х	Х

Legend: X - Listed '-' - Not Listed KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

#### 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

# Seveso III Directive (2012/18/EC)

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

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

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)
Ī	Trifluoroacetic acid	=	Listed	Listed	Listed	Listed

#### Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Revision Date 24-Mar-2024

(CAS #: 76-05-1)			

#### **PFAS Legend**

Listed = Meets the PFAS definition of the named authority

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at

Take note of Directive 2000/39/EC establishing a first list of indicative occupational exposure limit values

# **National Regulations**

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

#### **WGK Classification**

Water endangering class = 2 (self classification)

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Acetonitrile	WGK2	
Trifluoroacetic acid	WGK2	

Component	France - INRS (Tables of occupational diseases)	
Acetonitrile	Tableaux des maladies professionnelles (TMP) - RG 84	

#### **Swiss Regulations**

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

#### 15.2. Chemical safety assessment

Chemical Safety Assessment/Reports (CSA/CSR) are not required for mixtures

#### **SECTION 16: OTHER INFORMATION**

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

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H332 - Harmful if inhaled

H319 - Causes serious eye irritation

H225 - Highly flammable liquid and vapor

H314 - Causes severe skin burns and eye damage

H318 - Causes serious eye damage

H412 - Harmful to aquatic life with long lasting effects

EUH071 - Corrosive to the respiratory tract

#### Legend

**CAS** - Chemical Abstracts Service

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

**ENCS** - Japanese Existing and New Chemical Substances

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances **KECL** - Korean Existing and Evaluated Chemical Substances

**AICS** - Australian Inventory of Chemical Substances NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

Substances List

EC50 - Effective Concentration 50%

#### Acetonitrile with 0.1% Trifluoroacetic Acid (v/v), LC-MS

Revision Date 24-Mar-2024

NOEC - No Observed Effect ConcentrationPOW - Partition coefficient Octanol:WaterPBT - Persistent, Bioaccumulative, ToxicvPvB - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate
VOC - (volatile organic compound)

Key literature references and sources for data

https://echa.europa.eu/information-on-chemicals

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

# Classification and procedure used to derive the classification for mixtures according to Regulation (EC) 1272/2008 [CLP]:

Physical hazards
Health Hazards
Calculation method
Environmental hazards
Calculation method

#### **Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Prepared By Health, Safety and Environmental Department

**Creation Date** 09-Dec-2022 **Revision Date** 09-Dec-2022 24-Mar-2024

**Revision Summary** New emergency telephone response service provider.

# This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No. 1907/2006

For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2, Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and Preparations).

#### 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 Safety Data Sheet**