

## Safety Data Sheet

according to Regulation (EC) No 1907/2006

### Acetonitrile / water / trifluoroacetic acid (TFA) mixture mixed 90 : 9.9 : 0.1 volumetrically for li

Revision date: 22.08.2023

Product code: 18485

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#### SECTION 1: Identification of the substance/mixture and of the company/undertaking

##### 1.1. Product identifier

Acetonitrile / water / trifluoroacetic acid (TFA) mixture mixed 90 : 9.9 : 0.1 volumetrically for li

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

###### Use of the substance/mixture

Laboratory chemical

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

###### Uses advised against

Do not use for private purposes (household).

##### 1.3. Details of the supplier of the safety data sheet

Company name:	AnalytiChem GmbH	
Street:	Stempelstraße 6	
Place:	D-47167 Duisburg	
Telephone:	0203/5194-0	Telefax: 0203/5194-290
E-mail:	info@analytichem.de	
Contact person:	Abteilung Produktsicherheit	Telephone: 0203/5194-107/117
E-mail:	produktsicherheit@analytichem.de	
Internet:	www.analytichem.de	
Responsible Department:	Abteilung Produktsicherheit	

##### 1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

##### Further Information

This product is a mixture. REACH Registration Number see section 3.

#### SECTION 2: Hazards identification

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

###### Regulation (EC) No 1272/2008

Flam. Liq. 2; H225  
Acute Tox. 4; H302  
Acute Tox. 4; H312  
Acute Tox. 4; H332  
Eye Irrit. 2; H319

Full text of hazard statements: see SECTION 16.

##### 2.2. Label elements

###### Regulation (EC) No 1272/2008

Signal word: Danger

Pictograms:



###### Hazard statements

H225 Highly flammable liquid and vapour.  
H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.

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H319 Causes serious eye irritation.

**Precautionary statements**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
P240 Ground and bond container and receiving equipment.  
P302+P352 IF ON SKIN: Wash with plenty of soap and water.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

**2.3. Other hazards**

No information available.

**SECTION 3: Composition/information on ingredients**

**3.2. Mixtures**

**Hazardous components**

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
75-05-8	acetonitrile			90 - < 95 %
	200-835-2	608-001-00-3	01-2119471307-38	
	Flam. Liq. 2, Acute Tox. 4, Acute Tox. 4, Acute Tox. 4, Eye Irrit. 2; H225 H332 H312 H302 H319			

Full text of H and EUH statements: see section 16.

**Specific Conc. Limits, M-factors and ATE**

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
75-05-8	200-835-2	acetonitrile	90 - < 95 %
	inhalation: LC50 = 3587 mg/l (vapours); inhalation: ATE = 1,5 mg/l (dusts or mists); dermal: LD50 = > 2000 mg/kg; oral: LD50 = 469 mg/kg		

**Further Information**

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

**SECTION 4: First aid measures**

**4.1. Description of first aid measures**

**General information**

No data available

**After inhalation**

Provide fresh air. Call a physician immediately.  
If breathing is irregular or stopped, administer artificial respiration.

**After contact with skin**

Take off immediately all contaminated clothing and wash it before reuse.  
Call a physician immediately.

**After contact with eyes**

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

**After ingestion**

Rinse mouth immediately and drink plenty of water. Call a physician immediately.

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

Headache  
Dyspnoea  
Irritant  
Vomiting  
Spasms  
Unconsciousness  
Respiratory complaints  
Cardiac arrhythmias  
Dizziness  
Release of: Hydrogen cyanide (hydrocyanic acid)

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

No data available

### **SECTION 5: Firefighting measures**

#### **5.1. Extinguishing media**

##### **Suitable extinguishing media**

Water spray jet, Carbon dioxide (CO<sub>2</sub>), Foam, Extinguishing powder.

##### **Unsuitable extinguishing media**

no restriction

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

Combustible liquid.  
Vapours are heavier than air, spread along floors and form explosive mixtures with air.  
Hazardous combustion products  
In case of fire may be liberated:  
Carbon dioxide (CO<sub>2</sub>) Carbon monoxide  
Hydrogen cyanide (hydrocyanic acid)  
Hydrogen fluoride  
Beware of reignition.

#### **5.3. Advice for firefighters**

In case of fire: Wear self-contained breathing apparatus.  
In case of fire and/or explosion do not breathe fumes.  
Avoid contact with skin, eyes and clothes.

#### **Additional information**

Danger of bursting container.  
Use water spray jet to protect personnel and to cool endangered containers.  
Suppress gases/vapours/mists with water spray jet.  
Move undamaged containers from immediate hazard area if it can be done safely.

### **SECTION 6: Accidental release measures**

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

##### **General advice**

Keep away from sources of ignition - No smoking.  
This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).  
Take action to prevent static discharges.

##### **For non-emergency personnel**

Provide adequate ventilation.  
Use personal protection equipment.

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Avoid contact with skin, eyes and clothes.  
Remove persons to safety.  
Emergency procedures  
Do not breathe dust/fume/gas/mist/vapours/spray.

#### For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

#### 6.2. Environmental precautions

Do not allow to enter into surface water or drains.  
The vapour of the product is heavier than air and may accumulate below ground level, in pits, channels and basements in higher concentration.  
Danger of explosion

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

##### For containment

Cover drains.  
Prevent spread over a wide area (e.g. by containment or oil barriers).  
Collect in closed and suitable containers for disposal.  
Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

##### For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

##### Other information

Provide adequate ventilation.  
Do not breathe dust/fume/gas/mist/vapours/spray.  
Wear breathing apparatus if exposed to vapours/dusts/aerosols.

#### 6.4. Reference to other sections

Safe handling: see section 7  
Personal protection equipment: see section 8  
Disposal: see section 13

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Advice on safe handling

Read label before use. Handle and open container with care.  
When using do not eat, drink, smoke, sniff. Keep container tightly closed.  
Use personal protection equipment. Use extractor hood (laboratory).  
Do not breathe vapour/aerosol. Provide adequate ventilation.

#### Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.  
Vapours can form explosive mixtures with air.

#### Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.  
Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.

#### Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.  
Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary.  
If handled uncovered, arrangements with local exhaust ventilation have to be used.

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

#### Requirements for storage rooms and vessels

Keep container tightly closed. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks,

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open flames and other ignition sources. No smoking.  
storage temperature: +5°C - +30°C

**Further information on storage conditions**

Keep cool. Protect from sunlight.

**7.3. Specific end use(s)**

Laboratory chemicals

**SECTION 8: Exposure controls/personal protection**

**8.1. Control parameters**

**Occupational exposure limits**

CAS No	Substance	ppm	mg/m <sup>3</sup>	fib/cm <sup>3</sup>	Category	Origin
75-05-8	Acetonitrile	40	70		TWA (8 h)	

**DNEL/DMEL values**

CAS No	Substance	Exposure route	Effect	Value
75-05-8	acetonitrile			
	Worker DNEL, long-term	inhalation	systemic	68 mg/m <sup>3</sup>
	Worker DNEL, acute	inhalation	systemic	68 mg/m <sup>3</sup>
	Worker DNEL, long-term	inhalation	local	68 mg/m <sup>3</sup>
	Worker DNEL, acute	inhalation	local	68 mg/m <sup>3</sup>
	Worker DNEL, long-term	dermal	systemic	32,2 mg/kg bw/day
	Consumer DNEL, long-term	inhalation	systemic	4,8 mg/m <sup>3</sup>
	Consumer DNEL, acute	inhalation	systemic	220 mg/m <sup>3</sup>
	Consumer DNEL, long-term	inhalation	local	4,8 mg/m <sup>3</sup>
	Consumer DNEL, acute	inhalation	local	22 mg/m <sup>3</sup>
	Consumer DNEL, acute	oral	systemic	0,6 mg/kg bw/day

**PNEC values**

CAS No	Substance	Value
75-05-8	acetonitrile	
	Freshwater	10 mg/l
	Freshwater (intermittent releases)	10 mg/l
	Marine water	1 mg/l
	Freshwater sediment	7,53 mg/kg
	Micro-organisms in sewage treatment plants (STP)	32 mg/l
	Soil	2,41 mg/kg

**8.2. Exposure controls**

**Appropriate engineering controls**

Technical measures and the application of suitable work processes have priority over personal protection equipment.

If handled uncovered, arrangements with local exhaust ventilation have to be used.

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#### Individual protection measures, such as personal protective equipment

##### Eye/face protection

Suitable eye protection: goggles.

##### Hand protection

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: [vertrieb@kcl.de](mailto:vertrieb@kcl.de) With specification (test according to EN374):

By long-term hand contact

Trade name/designation KCL 897 Butoject®

Suitable material: Butyl caoutchouc (butyl rubber) 0,3 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation KCL 897 Butoject®

Suitable material: Butyl caoutchouc (butyl rubber) 0,3 mm

Wearing time with occasional contact (splashes): > 480 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. This recommendation applies only to the product stated in the safety data sheet (>, <) supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

##### Skin protection

Flame-retardant protective clothing. Wear anti-static footwear and clothing

##### Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

##### Environmental exposure controls

Do not allow to enter into surface water or drains.

Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.

Danger of explosion

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state:	Liquid	
Colour:	colourless	
Odour:	like: Ether	
Odour threshold:	No data available	
Melting point/freezing point:		No data available
Boiling point or initial boiling point and boiling range:		>35 °C
Flammability:		not applicable
Lower explosion limits:		No data available
Upper explosion limits:		No data available
Flash point:		<21 °C
Auto-ignition temperature:		No data available
Decomposition temperature:		not determined
pH-Value:		not determined
Viscosity / kinematic:		No data available

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Solubility in other solvents

not determined

Dissolution rate:

No data available

Partition coefficient n-octanol/water:

not determined

Dispersion stability:

No data available

Vapour pressure:

No data available

Vapour pressure:

No data available

Density:

0,80909 g/cm<sup>3</sup>

Relative density:

No data available

Bulk density:

No data available

Relative vapour density:

not determined

Particle characteristics:

No data available

#### 9.2. Other information

##### Information with regard to physical hazard classes

Explosive properties

Vapours may form explosive mixtures with air.

Sustaining combustion:

No data available

Self-ignition temperature

Solid:

not applicable

Gas:

not applicable

Oxidizing properties

Not oxidising.

##### Other safety characteristics

Evaporation rate:

not determined

Solvent separation test:

No data available

Solvent content:

No data available

Solid content:

No data available

Sublimation point:

No data available

Softening point:

No data available

Pour point:

No data available

No data available:

Viscosity / dynamic:

No data available

Flow time:

No data available

##### Further Information

No data available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Vapours may form explosive mixtures with air.

### 10.2. Chemical stability

Keep away from heat.

### 10.4. Conditions to avoid

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames. Vapours can form explosive mixtures with air.

### 10.5. Incompatible materials

Rubber articles

Plastic articles

### 10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

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**Further information**

No data available

**SECTION 11: Toxicological information**

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

**Toxicocinetics, metabolism and distribution**

There are no data available on the mixture itself.

**Acute toxicity**

Harmful if swallowed.  
Harmful in contact with skin.  
Harmful if inhaled.

**ATEmix calculated**

ATE (oral) > 2000 mg/kg; ATE (dermal) > 2000 mg/kg; ATE (inhalation vapour) > 20 mg/l; ATE (inhalation dust/mist) > 5 mg/l

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
75-05-8	acetonitrile				
	oral	LD50 469 mg/kg	Mouse	Study report (1998)	OECD Guideline 401
	dermal	LD50 > 2000 mg/kg	Rabbit	Study report (1997)	OECD Guideline 402
	inhalation (4 h) vapour	LC50 3587 mg/l	Mouse	Study report (1998)	OECD Guideline 403
	inhalation dust/mist	ATE 1,5 mg/l			

**Irritation and corrosivity**

Causes serious eye irritation.  
Skin corrosion/irritation: Based on available data, the classification criteria are not met.

**Sensitising effects**

Based on available data, the classification criteria are not met.

**Carcinogenic/mutagenic/toxic effects for reproduction**

Based on available data, the classification criteria are not met.

**STOT-single exposure**

Based on available data, the classification criteria are not met.

**STOT-repeated exposure**

Based on available data, the classification criteria are not met.

**Aspiration hazard**

Based on available data, the classification criteria are not met.

**Information on likely routes of exposure**

There are no data available on the mixture itself.

**Specific effects in experiment on an animal**

There are no data available on the mixture itself.

**Additional information on tests**

There are no data available on the mixture itself.

**Practical experience**

There are no data available on the mixture itself.

**11.2. Information on other hazards**



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**Endocrine disrupting properties**

There are no data available on the mixture itself.

**Other information**

There are no data available on the mixture itself.

**Further information**

Headache  
Dyspnoea  
Irritant  
Vomiting  
Spasms  
Unconsciousness  
Respiratory complaints  
Cardiac arrhythmias  
Dizziness  
Release of: Hydrogen cyanide (hydrocyanic acid)

**SECTION 12: Ecological information**

**12.1. Toxicity**

Based on available data, the classification criteria are not met.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h]   [d]	Species	Source	Method
75-05-8	acetonitrile					
	Acute fish toxicity	LC50 1640 mg/l	96 h	Pimephales promelas	Review article or handbook (1984)	Guideline not specified
	Acute algae toxicity	ErC50 3560 mg/l	72 h	Phaeodactylum tricorutum	Study report (2010)	ISO 10253
	Acute crustacea toxicity	EC50 3600 mg/l	48 h	Daphnia magna	Bull. Environ. Contam. Toxicol. 57:655-6	other: OECD Guidelines for Testing Chemi
	Fish toxicity	NOEC 102 mg/l	7 d	Oryzias latipes	Study report (1996)	OECD Guideline 204
	Crustacea toxicity	NOEC 960 mg/l	21 d	Daphnia magna	Study report (1996)	other: OECD Guideline 202

**12.2. Persistence and degradability**

There are no data available on the mixture itself.

**12.3. Bioaccumulative potential**

There are no data available on the mixture itself.

**Partition coefficient n-octanol/water**

CAS No	Chemical name	Log Pow
75-05-8	acetonitrile	0,29

**BCF**

CAS No	Chemical name	BCF	Species	Source
75-05-8	acetonitrile	3		HSDB (2009)

**12.4. Mobility in soil**

There are no data available on the mixture itself.

**12.5. Results of PBT and vPvB assessment**

The substances in the mixture do not meet the PBT/vPvB criteria according to REACH, annex XIII.

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#### **12.6. Endocrine disrupting properties**

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

#### **12.7. Other adverse effects**

There are no data available on the mixture itself.

#### **Further information**

There are no data available on the mixture itself.

### SECTION 13: Disposal considerations

#### **13.1. Waste treatment methods**

##### **Disposal recommendations**

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.  
Send to a physico-chemical treatment facility under observation of official regulations.  
Do not empty into drains.

##### **Contaminated packaging**

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

### SECTION 14: Transport information

#### **Land transport (ADR/RID)**

<b>14.1. UN number or ID number:</b>	UN 1648
<b>14.2. UN proper shipping name:</b>	ACETONITRILE
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	II
Hazard label:	3
Classification code:	F1
Limited quantity:	1 L
Excepted quantity:	E2
Transport category:	2
Hazard No:	33
Tunnel restriction code:	D/E

#### **Inland waterways transport (ADN)**

<b>14.1. UN number or ID number:</b>	UN 1648
<b>14.2. UN proper shipping name:</b>	ACETONITRILE
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	II
Hazard label:	3
Classification code:	F1
Limited quantity:	1 L
Excepted quantity:	E2

#### **Marine transport (IMDG)**

<b>14.1. UN number or ID number:</b>	UN 1648
<b>14.2. UN proper shipping name:</b>	ACETONITRILE
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	II
Hazard label:	3
Special Provisions:	-
Limited quantity:	1 L
Excepted quantity:	E2
EmS:	F-E, S-D

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**Air transport (ICAO-TI/IATA-DGR)**

<b>14.1. UN number or ID number:</b>	UN 1648	
<b>14.2. UN proper shipping name:</b>	ACETONITRILE	
<b>14.3. Transport hazard class(es):</b>	3	
<b>14.4. Packing group:</b>	II	
Hazard label:	3	
Limited quantity Passenger:	1 L	
Passenger LQ:	Y341	
Excepted quantity:	E2	
IATA-packing instructions - Passenger:		353
IATA-max. quantity - Passenger:		5 L
IATA-packing instructions - Cargo:		364
IATA-max. quantity - Cargo:		60 L

**14.5. Environmental hazards**

ENVIRONMENTALLY HAZARDOUS: No

**14.6. Special precautions for user**

Warning: Combustible liquid.

**14.7. Maritime transport in bulk according to IMO instruments**

not applicable

**SECTION 15: Regulatory information**

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

**EU regulatory information**

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40, Entry 75

Information according to 2012/18/EU (SEVESO III): P5c FLAMMABLE LIQUIDS

**National regulatory information**

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D): 2 - obviously hazardous to water

Skin resorption/Sensitization: Permeates easily through outer skin and causes poisoning.

**SECTION 16: Other information**

**Changes**

This data sheet contains changes from the previous version in section(s): 9,12.

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**Abbreviations and acronyms**

ADR: Accord européen sur le transport des marchandises dangereuses par Route  
(European Agreement concerning the International Carriage of Dangerous Goods by Road)  
IMDG: International Maritime Code for Dangerous Goods  
IATA: International Air Transport Association  
GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
EINECS: European Inventory of Existing Commercial Chemical Substances  
ELINCS: European List of Notified Chemical Substances  
CAS: Chemical Abstracts Service  
LC50: Lethal concentration, 50%  
LD50: Lethal dose, 50%  
Flam. Liq: Flammable liquid  
Acute Tox: Acute toxicity  
Eye Irrit: Eye irritation

**Classification for mixtures and used evaluation method according to Regulation (EC) No 1272/2008 [CLP]**

Classification	Classification procedure
Flam. Liq. 2; H225	On basis of test data
Acute Tox. 4; H302	Calculation method
Acute Tox. 4; H312	Calculation method
Acute Tox. 4; H332	Calculation method
Eye Irrit. 2; H319	Calculation method

**Relevant H and EUH statements (number and full text)**

H225 Highly flammable liquid and vapour.  
H302 Harmful if swallowed.  
H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.  
H312 Harmful in contact with skin.  
H319 Causes serious eye irritation.  
H332 Harmful if inhaled.

**Further Information**

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.

*(The data for the hazardous ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)*