

Trifluoroacetic acid for LC-MS

Version number: GHS 1.0

Date of compilation: 2022-11-22

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

1.1 Product identifier

Identification of the substance	Trifluoroacetic acid for LC-MS
CAS number	76-05-1
Article number	LC-11105

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

Relevant identified uses	General use
Uses advised against	Do not use for squirting or spraying. Do not use for products which come into direct contact with the skin.

1.3 Details of the supplier of the safety data sheet

NeoFroxx GmbH
Marie-Curie-Str. 3
D-64683 Einhausen
Germany

Telephone: +49 (6251) 989 24 - 0
e-mail: info@neofroxx.com
Website: neofroxx.com

e-mail (competent person) info@neofroxx.com (neoFroxx GmbH)

1.4 Emergency telephone number

Poison centre			
Country	Name	Postal code/city	Telephone
United Kingdom	National Poisons Information Service		111

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Category	Hazard class and category	Hazard statement
3.1I	acute toxicity (inhal.)	4	Acute Tox. 4	H332
3.2	skin corrosion/irritation	1A	Skin Corr. 1A	H314
3.3	serious eye damage/eye irritation	1	Eye Dam. 1	H318
4.1C	hazardous to the aquatic environment - chronic hazard	3	Aquatic Chronic 3	H412

For full text of abbreviations: see SECTION 16.

The most important adverse physicochemical, human health and environmental effects

Skin corrosion produces an irreversible damage to the skin; namely, visible necrosis through the epidermis and into the dermis. Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

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Labelling

- Signal word danger

- Pictograms

GHS05, GHS07



- Hazard statements

H314 Causes severe skin burns and eye damage.
H332 Harmful if inhaled.
H412 Harmful to aquatic life with long lasting effects.

- Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P273 Avoid release to the environment.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P301+P330+P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310 Immediately call a POISON CENTER/doctor.
P501 Dispose of contents/container to industrial combustion plant.

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Trifluoroacetic acid for LC-MS

Identifiers

CAS No 76-05-1
EC No 200-929-3
Index No 607-091-00-1
(GB CLP)

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	11 mg/l/4h	inhalation: vapour

Molecular formula C₂HF₃O₂

Molar mass 114 g/mol

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SECTION 4: First aid measures

4.1 Description of first aid measures

General notes

Do not leave affected person unattended. Remove victim out of the danger area. Keep affected person warm, still and covered. Take off immediately all contaminated clothing. In all cases of doubt, or when symptoms persist, seek medical advice. In case of unconsciousness place person in the recovery position. Never give anything by mouth.

Following inhalation

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions. In case of respiratory tract irritation, consult a physician. Provide fresh air.

Following skin contact

Wash with plenty of soap and water.

Following eye contact

Remove contact lenses, if present and easy to do. Continue rinsing. Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart.

Following ingestion

Rinse mouth with water (only if the person is conscious). Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water spray, Alcohol resistant foam, BC-powder, Carbon dioxide (CO₂)

Unsuitable extinguishing media

Water jet

5.2 Special hazards arising from the substance or mixture

Hazardous combustion products

Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Co-ordinate firefighting measures to the fire surroundings. Do not allow firefighting water to enter drains or water courses. Collect contaminated firefighting water separately. Fight fire with normal precautions from a reasonable distance.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Remove persons to safety.

For emergency responders

Wear breathing apparatus if exposed to vapours/dust/spray/gases.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

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6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains

Advice on how to clean up a spill

Wipe up with absorbent material (e.g. cloth, fleece). Collect spillage: sawdust, kieselgur (diatomite), sand, universal binder

Appropriate containment techniques

Use of adsorbent materials.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Recommendations

- Measures to prevent fire as well as aerosol and dust generation
Use local and general ventilation. Use only in well-ventilated areas.
- Handling of incompatible substances or mixtures
Do not mix with alkali.
- Keep away from
Caustic solutions

Advice on general occupational hygiene

Wash hands after use. Do not eat, drink and smoke in work areas. Remove contaminated clothing and protective equipment before entering eating areas. Never keep food or drink in the vicinity of chemicals. Never place chemicals in containers that are normally used for food or drink. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

- Ventilation requirements
Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted.
- Packaging compatibilities
Only packagings which are approved (e.g. acc. to ADR) may be used.

7.3 Specific end use(s)

See section 16 for a general overview.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

This information is not available.

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Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	2.67 mg/m ³	human, inhalatory	worker (industry)	chronic - local effects
DNEL	16 mg/m ³	human, inhalatory	worker (industry)	acute - local effects

Environmental values

Relevant PNECs and other threshold levels				
Endpoint	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0.56 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.056 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	83.2 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	2.36 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.236 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	4.7 µg/kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Appropriate engineering controls

General ventilation.

Individual protection measures (personal protective equipment)

Eye/face protection

Wear eye/face protection.

Skin protection

- Hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. In the case of wanting to use the gloves again, clean them before taking off and air them well. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

- Type of material

NBR: acrylonitrile-butadiene rubber

- Material thickness

min. 0,7 mm

- Breakthrough times of the glove material

>480 minutes (permeation: level 6)

- Other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended. Wash hands thoroughly after handling.

Respiratory protection

P2 (filters at least 94 % of airborne particles, colour code: White).

Environmental exposure controls

Use appropriate container to avoid environmental contamination. Keep away from drains, surface and ground water.

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SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	stinging
Melting point/freezing point	-15.2 °C
Boiling point or initial boiling point and boiling range	71.78 °C at 1,013 hPa
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	>100 °C at 101.3 kPa
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	1 (in aqueous solution: 10 g/l, 20 °C) (acid)
Kinematic viscosity	not determined

Solubility(ies)

Water solubility	>10 g/cm ³
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Partition coefficient

Partition coefficient n-octanol/water (log value)	this information is not available
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Vapour pressure	12.4 kPa at 20 °C
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Density and/or relative density

Density	1.479 g/cm ³ at 24.77 °C
Relative vapour density	information on this property is not available

Particle characteristics	not relevant (liquid)
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9.2 Other information

Information with regard to physical hazard classes	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics	
Surface tension	72.5 mN/m (20 °C) (ECHA)

SECTION 10: Stability and reactivity

10.1 Reactivity

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials".

10.2 Chemical stability

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

No known hazardous reactions.

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

Oxidisers

10.6 Hazardous decomposition products

Reasonably anticipated hazardous decomposition products produced as a result of use, storage, spill and heating are not known. Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if inhaled.

- Acute toxicity estimate (ATE)

Inhalation: vapour 11 mg/l/4h

Skin corrosion/irritation

Causes severe skin burns and eye damage.

Serious eye damage/eye irritation

Causes serious eye damage.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

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Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

11.2 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

Aquatic toxicity (chronic)			
Endpoint	Value	Species	Exposure time
EC50	>100 mg/l	aquatic invertebrates	21 d

12.2 Persistence and degradability

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	0 %	28 d

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. Completely emptied packages can be recycled. Handle contaminated packages in the same way as the substance itself.

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Remarks

Please consider the relevant national or regional provisions. Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities.

SECTION 14: Transport information

14.1 UN number or ID number

ADR/RID	UN 2699
IMDG-Code	UN 2699
ICAO-TI	UN 2699

14.2 UN proper shipping name

ADR/RID	TRIFLUOROACETIC ACID
IMDG-Code	TRIFLUOROACETIC ACID
ICAO-TI	Trifluoroacetic acid

14.3 Transport hazard class(es)

ADR/RID	8
IMDG-Code	8
ICAO-TI	8

14.4 Packing group

ADR/RID	I
IMDG-Code	I
ICAO-TI	I

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

Information for each of the UN Model Regulations

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR) - Additional information

Classification code	C3
Danger label(s)	8



Excepted quantities (EQ)	E0
Limited quantities (LQ)	0
Transport category (TC)	1
Tunnel restriction code (TRC)	E
Hazard identification No	88

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Emergency Action Code	2X
Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) - Additional information	
Classification code	C3
Danger label(s)	8
	
Excepted quantities (EQ)	E0
Limited quantities (LQ)	0
Transport category (TC)	1
Hazard identification No	88
International Maritime Dangerous Goods Code (IMDG) - Additional information	
Marine pollutant	-
Danger label(s)	8
	
Excepted quantities (EQ)	E0
Limited quantities (LQ)	0
EmS	F-A, S-B
Stowage category	B
Segregation group	1 - Acids
International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information	
Danger label(s)	8
	
Excepted quantities (EQ)	E0

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture Relevant provisions of the European Union (EU)

Deco-Paint Directive

VOC content	100 %
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Industrial Emissions Directive (IED)

VOC content	100 %
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Water Framework Directive (WFD)

List of pollutants (WFD)			
Name of substance	CAS No	Listed in	Remarks
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Legend

A) Indicative list of the main pollutants

Regulation on persistent organic pollutants (POP)

Not listed.

National regulations (GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
Trifluoroacetic acid for LC-MS	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3

National inventories

Country	Inventory	Status
EU	REACH Reg.	substance is listed
US	TSCA	substance is listed

Legend

REACH Reg. REACH registered substances
TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval

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Abbr.	Descriptions of used abbreviations
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GB CLP	The Chemicals (Health and Safety) and Genetically Modified Organisms (Contained Use) (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/720 (as amended)
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
index No	The Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H332	Harmful if inhaled.
H412	Harmful to aquatic life with long lasting effects.

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Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product. The information is intended to give you guidelines for the safe handling of the product mentioned in this safety data sheet during storage, processing, transport and disposal. The information is not transferable to other products. Insofar as the product is mixed, blended or processed with other materials or is subjected to processing, the information in this safety data sheet cannot be transferred to the new material produced in this way, unless expressly stated otherwise.