

Safety data sheet

acc. to Safe Work Australia - Code of Practice



Trifluoroacetic acid (TFA) PEPTIPURE® ≥99,9 %, for peptide synthesis

article number: **P088**
Version: **GHS 4.0 en**
Replaces version of: 2022-01-19
Version: (GHS 3)

date of compilation: 2019-12-13
Revision: 2024-03-02

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

1.1 Product identifier

Identification of the substance	Trifluoroacetic acid (TFA) PEPTIPURE® ≥99,9 %, for peptide synthesis
Article number	P088
CAS number	76-05-1

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for squirting or spraying. Do not use for products which come into direct contact with the skin. Do not use for private purposes (household). Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone:+49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

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
2.16	Substance or mixture corrosive to metals	1	Met. Corr. 1	H290
3.1I	Acute toxicity (inhal.)	4	Acute Tox. 4	H332
3.2	Skin corrosion/irritation	1	Skin Corr. 1	H314
3.3	Serious eye damage/eye irritation	1	Eye Dam. 1	H318

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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.

2.2 Label elements

Labelling

Signal word

Danger

Pictograms

GHS05, GHS07



Hazard statements

H290	May be corrosive to metals
H314	Causes severe skin burns and eye damage
H332	Harmful if inhaled

Precautionary statements

Precautionary statements - prevention

P260	Do not breathe dusts or mists
P280	Wear eye protection/face protection

Precautionary statements - response

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
P390	Absorb spillage to prevent material damage

Precautionary statements - disposal

P501	Dispose of contents/container to industrial combustion plant
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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.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Trifluoroacetic acid (TFA)
Molecular formula	C ₂ HF ₃ O ₂
Molar mass	114 g/mol
CAS No	76-05-1

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off immediately all contaminated clothing. Self-protection of the first aider.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

After contact with skin, wash immediately with plenty of water. Immediate medical treatment required because corrosive injuries that are not treated are hard to cure.

Following eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye.

Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately. If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects).

4.2 Most important symptoms and effects, both acute and delayed

Corrosion, Gastric perforation, Nausea, Vomiting, Unconsciousness, Headache, Circulatory collapse, Dyspnoea, Pulmonary oedema, Risk of serious damage to eyes, Risk of blindness

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!

water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

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Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. 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 monoxide (CO), Carbon dioxide (CO₂), Hydrogen fluoride (HF)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. The product is an acid. Before discharge into sewage plants the product normally needs to be neutralised.

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

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

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

Provision of sufficient ventilation. Use extractor hood (laboratory). Handle and open container with care. Clear contaminated areas thoroughly.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep container tightly closed. Hygroscopic.

Incompatible substances or mixtures

Observe hints for combined storage.

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Protect against external exposure, such as

high temperatures, humidity

Consideration of other advice:

Ventilation requirements

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

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				
End-point	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

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Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection. Wear 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. 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. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

Butyl caoutchouc (butyl rubber)

• material thickness

≥0,5 mm

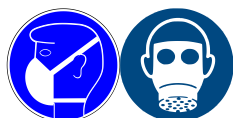
• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: B-P2 (combined filters for acidic gases and particles, colour code: Grey/White).

Environmental exposure controls

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 (ECHA)
Boiling point or initial boiling point and boiling range	71.78 °C at 1,013 hPa (ECHA)
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 (ECHA)
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	1 (in aqueous solution: 10 g/l, 20 °C) (ECHA)
Kinematic viscosity	not determined
Dynamic viscosity	0.9 – 9 mPa s at 20 °C
<u>Solubility(ies)</u>	
Water solubility	1,520 g/l at 20 °C (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	0.5 (ECHA)
Vapour pressure	12.4 kPa at 20 °C
<u>Density and/or relative density</u>	
Density	1.479 g/cm ³ at 24.77 °C (ECHA)
Relative vapour density	3.94 (air = 1)
Particle characteristics	not relevant (liquid)

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard classes:

Corrosive to metals category 1: corrosive to metals

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Other safety characteristics:

Surface tension

72.5 mN/m (20 °C) (ECHA)

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Substance or mixture corrosive to metals.

If heated

Vapours may form explosive mixtures with air.

10.2 Chemical stability

Moisture-sensitive.

10.3 Possibility of hazardous reactions

Violent reaction with: Alkali (lye), Ammonia (NH₃),

Dangerous/dangerous reactions with: Acids,

Danger of explosion: Hydrides

10.4 Conditions to avoid

Protect from moisture. Keep away from heat.

10.5 Incompatible materials

different plastics, different metals

Release of toxic materials with

Acids.

10.6 Hazardous decomposition products

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.

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.

Symptoms related to the physical, chemical and toxicological characteristics

- **If swallowed**

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects)

- **If in eyes**

causes burns, Causes serious eye damage, risk of blindness

- **If inhaled**

irritant effects, cough, pain, choking, and breathing difficulties

- **If on skin**

causes severe burns, causes poorly healing wounds

- **Other information**

Other adverse effects: Renal impairment, Circulatory collapse, Headache, Unconsciousness

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	>999 mg/l	fish	ECHA	96 h
EC50	>999 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	237.1 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	>25 mg/l	aquatic invertebrates	ECHA	21 d

12.2 Persistence and degradability

Theoretical Oxygen Demand: 0.3508 mg/mg
 Theoretical Carbon Dioxide: 0.7719 mg/mg

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

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	0.5 (ECHA)
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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

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

Relevant provisions relating to waste(Basel Convention)

Properties of waste which render it hazardous

H8 Corrosives

13.3 Remarks

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

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SECTION 14: Transport information

14.1 UN number

UN RTDG	UN 2699
IMDG-Code	UN 2699
ICAO-TI	UN 2699

14.2 UN proper shipping name

UN RTDG	TRIFLUOROACETIC ACID
IMDG-Code	TRIFLUOROACETIC ACID
ICAO-TI	Trifluoroacetic acid

14.3 Transport hazard class(es)

UN RTDG	8
IMDG-Code	8
ICAO-TI	8

14.4 Packing group

UN RTDG	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


There is no additional information.

14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Transport information National regulations Additional information(UN RTDG)

UN number	2699
Class	8
Packing group	I
Danger label(s)	8
	
Special provisions (SP)	- UN RTDG
Excepted quantities (EQ)	E0 UN RTDG
Limited quantities (LQ)	0 UN RTDG



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Emergency Action Code	2X
International Maritime Dangerous Goods Code (IMDG) - Additional information	
Proper shipping name	TRIFLUOROACETIC ACID
Particulars in the shipper's declaration	UN2699, TRIFLUOROACETIC ACID, 8, I
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	
Proper shipping name	Trifluoroacetic acid
Particulars in the shipper's declaration	UN2699, Trifluoroacetic acid, 8, I
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

There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed

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Country	Inventory	Status
JP	CSCL-ENCS	substance is listed
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC	Australian Inventory of Industrial Chemicals
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
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

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8		Emergency Action Code: 2X	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
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
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
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
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. 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
H290	May be corrosive to metals.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H332	Harmful if inhaled.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.