

Water with 0.1 % trifluoroacetic acid ROTISOLV® LC-MS-Grade

article number: CP05 date of compilation: 17.05.2021

Version: 1.0 en

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

1.1 **Product identifier**

Identification of the substance Water with 0.1 % trifluoroacetic acid ROT-

ISOLV® LC-MS-Grade

Article number CP05

Registration number (REACH) C, not relevant (mixture), It is not required to list

the identified uses because the substance is not subject to registration according to REACH (< 1 t/

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 products which come into contact

with foodstuffs. Do not use for private purposes

(household).

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 :Department Health, Safety and Environment

sheet:

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

1.4 **Emergency telephone number**

SECTION 2: Hazards identification

Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

This mixture does not meet the criteria for classification in accordance with Regulation No 1272/2008/ EC.

2.2 **Label elements**

Labelling according to Regulation (EC) No 1272/2008 (CLP)

not required

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2.3 Other hazards

Results of PBT and vPvB assessment

This mixture does not contain any substances that are assessed to be a PBT or a vPvB.

SECTION 3: Composition/information on ingredients

3.1 Substances

not relevant (mixture)

REACH Reg. No

C

3.2 Mixtures

Description of the mixture

Name of sub- stance	Identifier	Wt%	Classification acc. to GHS	Pictograms	Notes
Trifluoroacetic acid (TFA)	CAS No 76-05-1 EC No 200-929-3 Index No 607-091-00-1	0,1	Met. Corr. 1 / H290 Acute Tox. 4 / H332 Skin Corr. 1A / H314 Eye Dam. 1 / H318 Aquatic Chronic 3 / H412		B(a) GHS-HC

Notes

B(a): The classification refers to an aqueous solution

GHS-HC: Harmonised classification (the classification of the substance corresponds to the entry in the list according to 1272/2008/EC, Annex VI)

Name of sub- stance	Identifier	Specific Conc. Limits	M-Factors	ATE	Exposure route
Trifluoroacetic acid (TFA)	CAS No 76-05-1	-	-	11 ^{mg} / _l /4h	inhalation: va- pour
	EC No 200-929-3				
	Index No 607-091-00-1				

For full text of abbreviations: see SECTION 16

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air.

Following skin contact

Rinse skin with water/shower.

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Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

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

co-ordinate firefighting measures to the fire surroundings water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Ingredients of the mixture combustible. The product itself does not burn.

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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

No special measures are necessary.

6.2 Environmental precautions

Keep away from drains, surface and ground water.

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).

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Other information relating to spills and releases

Place in appropriate containers for disposal.

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

No special measures are necessary.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

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)

Data are not available.

Relevant DNELs of components of the mixture

Name of sub- stance	CAS No	End- point	Threshol d level	Protection goal, route of exposure	Used in	Exposure time
Trifluoroacetic acid (TFA)	76-05-1	DNEL	2,67 mg/ m³	human, inhalat- ory	worker (industry)	chronic - local ef- fects
Trifluoroacetic acid (TFA)	76-05-1	DNEL	16 mg/m ³	human, inhalat- ory	worker (industry)	acute - local ef- fects

Relevant PNECs of components of the mixture

Name of sub- stance	CAS No	End- point	Threshol d level	Organism	Environmental compartment	Exposure time
Trifluoroacetic acid (TFA)	76-05-1	PNEC	0,56 ^{mg} / _l	aquatic organ- isms	freshwater	short-term (single instance)
Trifluoroacetic acid (TFA)	76-05-1	PNEC	0,056 ^{mg} / _l	aquatic organ- isms	marine water	short-term (single instance)

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Relevant PNECs of components of the mixture Name of sub-**CAS No** End-**Threshol Organism Environmental Exposure time** stance d level point compartment 83,2 ^{mg}/_I Trifluoroacetic acid 76-05-1 **PNEC** aquatic organsewage treatment short-term (single (TFA) isms plant (STP) instance) 2,36 ^{mg}/_{kq} aquatic organ-Trifluoroacetic acid 76-05-1 **PNEC** freshwater sedishort-term (single instance) (TFA) isms ment Trifluoroacetic acid 0,236 mg/ aquatic organ-76-05-1 **PNEC** marine sediment short-term (single (TFA) isms instance) kg $4,7 \, ^{\mu g}/_{kg}$ Trifluoroacetic acid 76-05-1 **PNEC** terrestrial organsoil short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection





Use safety goggle with side protection.

Skin protection





hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

type of material

NBR (Nitrile rubber)

material thickness

>0,11 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: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

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Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state liquid

Colour colourless
Odour odourless

Melting point/freezing point 0 °C

Boiling point or initial boiling point and boiling 100 °C

range

Flammability non-combustible
Lower and upper explosion limit not determined
Flash point not determined
Auto-ignition temperature not determined
Decomposition temperature not relevant
pH (value) not determined

pH (value) not determined
Kinematic viscosity not determined

Solubility(ies)

Water solubility miscible in any proportion

Partition coefficient

Partition coefficient n-octanol/water (log value): this information is not available

Vapour pressure not determined

Density 1,001 g/_{cm³} at 20 °C

Relative vapour density information on this property is not available

Particle characteristics not relevant (liquid)

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard hazard classes acc. to GHS

classes: (physical hazards): not relevant

Other safety characteristics:

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Miscibility

completely miscible with water

SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: Alkaline earth metal, Alkali metals, Carbide, Strong acid

10.4 Conditions to avoid

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

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

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

Test data are not available for the complete mixture.

Classification procedure

The method for classification of the mixture is based on ingredients of the mixture (additivity formula).

Classification according to GHS (1272/2008/EC, CLP)

This mixture does not meet the criteria for classification in accordance with Regulation No 1272/2008/ EC.

Acute toxicity

Shall not be classified as acutely toxic.

Acute toxicity estimate (ATE) of components of the mixture

Name of substance	CAS No	Exposure route	ATE
Trifluoroacetic acid (TFA)	76-05-1	inhalation: vapour	11 ^{mg} / _l /4h

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

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.

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Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

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

Data are not available.

If in eyes

Data are not available.

If inhaled

Data are not available.

• If on skin

Data are not available.

Other information

Health effects are not known.

11.2 Endocrine disrupting properties

None of the ingredients are listed.

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute) of components of the mixture								
Name of sub- stance	CAS No	Endpoint	Value	Species	Exposure time			
Trifluoroacetic acid (TFA)	76-05-1	LC50	>999 ^{mg} / _l	fish	96 h			
Trifluoroacetic acid (TFA)	76-05-1	EC50	>999 ^{mg} / _l	aquatic invertebrates	48 h			
Trifluoroacetic acid (TFA)	76-05-1	ErC50	237,1 ^{mg} / _l	algae	72 h			

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Aquatic toxicity (chronic) of components of the mixture

Name of sub- stance	CAS No	Endpoint	Value	Species	Exposure time
Trifluoroacetic acid (TFA)	76-05-1	EC50	>25 ^{mg} / _l	aquatic invertebrates	21 d

Biodegradation

Data are not available.

12.2 Process of degradability

Degradability of components of the mixture

Name of substance	CAS No	Process	Degrada- tion rate	Time	Method	Source
Trifluoroacetic acid (TFA)	76-05-1	oxygen deple- tion	0 %	28 d		ECHA

12.3 Bioaccumulative potential

Data are not available.

Bioaccumulative potential of components of the mixture

Name of substance	CAS No	BCF	Log KOW	BOD5/COD
Trifluoroacetic acid (TFA)	76-05-1		0,5	

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

None of the ingredients are listed.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

Sewage disposal-relevant information

Do not empty into drains.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process. Waste catalogue ordinance (Germany).

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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.

SECTION 14: Transport information

14.1 UN number or ID number not subject	to transport regulations
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14.2 UN proper shipping name not assigned

Transport hazard class(es) 14.3 none

Packing group not assigned 14.4

Environmental hazards non-environmentally hazardous acc. to the dan-14.5

gerous goods regulations

14.6 Special precautions for user

There is no additional information.

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 14.8

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information

Not subject to ADR, RID and ADN.

International Maritime Dangerous Goods Code (IMDG) - Additional information

Not subject to IMDG.

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Not subject to ICAO-IATA.

SECTION 15: Regulatory information

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

Restrictions according to REACH, Annex XVII

Dangerous substances with restrictions (REACH, Annex XVII)

Name of substance	Name acc. to inventory	CAS No	Restriction	No
Trifluoroacetic acid (TFA)	this product meets the criteria for classification in accordance with Reg- ulation No 1272/2008/EC		R3	3

Legend

1. Shall not be used in:

ornamental articles intended to produce light or colour effects by means of different phases, for example in ornamental lamps and ashtrays,

- tricks and jokes,

- games for one or more participants, or any article intended to be used as such, even with ornamental aspects, 2. Articles not complying with paragraph 1 shall not be placed on the market.

3. Shall not be placed on the market if they contain a colouring agent, unless required for fiscal reasons, or perfume,

— can be used as fuel in decorative oil lamps for supply to the general public, and
— present an aspiration hazard and are labelled with H304.

4. Decorative oil lamps for supply to the general public shall not be placed on the market unless they conform to the European Standard on Decorative oil lamps (EN 14059) adopted by the European Committee for Standardisation

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Legend

(CEN).
5. Without prejudice to the implementation of other Union provisions relating to the classification, labelling and packaging of substances and mixtures, suppliers shall ensure, before the placing on the market, that the following require-

(a) lamp oils, labelled with H304, intended for supply to the general public are visibly, legibly and indelibly marked as follows: "Keep lamps filled with this liquid out of the reach of children"; and, by 1 December 2010, "Just a sip of lamp oil – or even sucking the wick of lamps – may lead to life-threatening lung damage";

(c) lamps oils and grill lighters, labelled with H304, intended for supply to the general public are legibly and indelibly marked by 1 December 2010 as follows: 'Just a sip of grill lighter fluid may lead to life threatening lung damage'; (c) lamps oils and grill lighters, labelled with H304, intended for supply to the general public are packaged in black opaque containers not exceeding 1 litre by 1 December 2010.';

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

None of the ingredients are listed. (Or Concentration of the substance in a mixture: <0.1 % Mass concentration)

Seveso Directive

2012/	18/EU (Seveso III)						
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes				
	not assigned						

Deco-Paint Directive

VOC content	0,1 % -405,6 ^g / _I
	1.00/6 /1

Industrial Emissions Directive (IED)

VOC content	0,1 %
VOC content Water content was discounted	-405,6 ^g / _l

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

none of the ingredients are listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

none of the ingredients are listed

Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
Trifluoroacetic acid (TFA)	Organohalogen compounds and substances which may form such compounds in the aquatic envir- onment		A)	

Legend

Indicative list of the main pollutants

Regulation on the marketing and use of explosives precursors

none of the ingredients are listed

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Regulation on drug precursors

none of the ingredients are listed

Regulation on substances that deplete the ozone layer (ODS)

none of the ingredients are listed

Regulation concerning the export and import of hazardous chemicals (PIC)

none of the ingredients are listed

Regulation on persistent organic pollutants (POP)

none of the ingredients are listed

National inventories

Country	Inventory	Status
AU	AICS	all ingredients are listed
CA	DSL	all ingredients are listed
CN	IECSC	all ingredients are listed
EU	ECSI	all ingredients are listed
EU	REACH Reg.	all ingredients are listed
JP	CSCL-ENCS	all ingredients are listed
JP	ISHA-ENCS	not all ingredients are listed
KR	KECI	all ingredients are listed
MX	INSQ	all ingredients are listed
NZ	NZIoC	all ingredients are listed
PH	PICCS	all ingredients are listed
TW	TCSI	all ingredients are listed
US	TSCA	all ingredients are listed

Legend

AICS CSCL-ENCS

DSL ECSI IECSC INSQ

Australian Inventory of Chemical Substances
List of Existing and New Chemical Substances (CSCL-ENCS)
Domestic Substances List (DSL)
EC Substance Inventory (EINECS, ELINCS, NLP)
Inventory of Existing Chemical Substances Produced or Imported in China National Inventory of Chemical Substances
Inventory of Existing and New Chemical Substances (ISHA-ENCS)
Korea Existing Chemicals Inventory
New Zealand Inventory of Chemicals
Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH registered substances

ISHA-ENCS

KECI

REACH Reg. REACH registered substances
TCSI Taiwan Chemical Substance Inventory
TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

Chemical safety assessments for substances in this mixture were not carried out.

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SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
Acute Tox.	Acute toxicity
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de naviga- tion intérieures (European Agreement concerning the International Carriage of Dangerous Goods by In- land Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
Aquatic Chronic	Hazardous to the aquatic environment - chronic hazard
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
BOD	Biochemical Oxygen Demand
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
COD	Chemical oxygen demand
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
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
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
Eye Dam.	Seriously damaging to the eye
Eye Irrit.	Irritant to the eye
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
IMDG	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
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
log KOW	n-Octanol/water
Met. Corr.	Substance or mixture corrosive to metals

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Abbr.	Descriptions of used abbreviations
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)
Skin Corr.	Corrosive to skin
Skin Irrit.	Irritant to skin
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

Classification procedure

Physical and chemical properties. The classification is based on tested mixture. Health hazards. Environmental hazards. The method for classification of the mixture is based on ingredients of the mixture (additivity formula).

List of relevant phrases (code and full text as stated in chapter 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.
H412	Harmful to aquatic life with long lasting effects.

Disclaimer

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

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