according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

article number: **CP02** Version: **2.0 en** Replaces version of: 2021-08-27 Version: (1)

date of compilation: 2021-08-27 Revision: 2024-03-04

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

CP02

608-001-00-3

200-835-2

75-05-8

#### 1.1 Product identifier

Identification of the substance

Article number

Registration number (REACH) Index number in CLP Annex VI EC number

CAS number

#### **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 private purposes (household). Food, drink and animal feedingstuffs.

Acetonitrile with 0,1 % Trifluoroacetic acid

ROTISOLV® ≥99,9 %, LC-MS Grade

01-2119471307-38-xxxx

#### 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:

#### e-mail (competent person):

#### sicherheit@carlroth.de

#### 1.4 Emergency telephone number

| Name  | Street        | Postal<br>code/city | Telephone       | Website                     |
|---|---------------|---------------------|-----------------|-----------------------------|
| National Poisons Information<br>Centre<br>Beaumont Hospital | Beaumont Road | Dublin 9            | +353 1 809 2166 | https://<br>www.poisons.ie/ |

### **SECTION 2: Hazards identification**

#### 2.1 Classification of the substance or mixture

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV $\circledast \geq \!\! 99,9$ %, LC-MS Grade

article number: CP02

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

| Section | Hazard class                      | Cat-<br>egory | Hazard class and category | Hazard<br>statement |
|---------|-----------------------------------|---------------|---------------------------|---------------------|
| 2.6     | Flammable liquid                  | 2             | Flam. Liq. 2              | H225                |
| 3.10    | Acute toxicity (oral)             | 4             | Acute Tox. 4              | H302                |
| 3.1D    | Acute toxicity (dermal)           | 4             | Acute Tox. 4              | H312                |
| 3.1I    | Acute toxicity (inhal.)           | 4             | Acute Tox. 4              | H332                |
| 3.3     | Serious eye damage/eye irritation | 2             | Eye Irrit. 2              | H319                |

For full text of abbreviations: see SECTION 16

#### The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

#### 2.2 Label elements

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

Signal word Danger

#### **Pictograms**

GHS02, GHS07



#### Hazard statements

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

#### **Precautionary statements**

#### **Precautionary statements - prevention**

| P210 | Keep away from heat, hot surfaces, sparks, open flames and other ignition |
|------|---|
|      | sources. No smoking   |
| P280 | Wear protective gloves/protective clothing/eye protection/face protection |

#### **Precautionary statements - response**

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

#### **Precautionary statements - storage**

P403+P235 Store in a well-ventilated place. Keep cool

#### Labelling of packages where the contents do not exceed 125 ml

Signal word: Danger





according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU

#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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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  $\ge 0,1\%$ .

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

| 3.1      | Substances |
|----------|------------|
| <b>U</b> | Jubblunces |

| Name of substance | Acetonitrile with 0,1 % Trifluoroacetic acid |
|-------------------|--|
| Molecular formula | $C_2H_3N$                                    |
| Molar mass        | 41,05 <sup>g</sup> / <sub>mol</sub>          |
| REACH Reg. No     | 01-2119471307-38-xxxx                        |
| CAS No            | 75-05-8                                      |
| EC No             | 200-835-2                                    |
| Index No          | 608-001-00-3                                 |

#### Impurities/additives/constituents:

| Name of substance          | Identifier               | Wt% |
|----------------------------|--------------------------|-----|
| Trifluoroacetic acid (TFA) | CAS No<br>76-05-1        | 0,1 |
|                            | EC No<br>200-929-3       |     |
|                            | Index No<br>607-091-00-1 |     |

| Substance, Specific Conc. Limits, M-factors, ATE   |   |   |                                      |  |  |  |  |
|--|---|---|--------------------------------------|--|--|--|--|
| Specific Conc. Limits M-Factors ATE Exposure route |   |   |                                      |  |  |  |  |
| -  | - | 469 <sup>mg</sup> / <sub>kg</sub><br>1.100 <sup>mg</sup> / <sub>kg</sub><br>11 <sup>mg</sup> / <sub>l</sub> /4h | oral<br>dermal<br>inhalation: vapour |  |  |  |  |

#### Remarks

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.



according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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#### Following inhalation

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

#### Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

#### **Following ingestion**

Rinse mouth with water (only if the person is conscious). Call a doctor.

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

After eye contact: Irritant effects, Conjunctival redness of the eyes, Following skin contact: Localised redness, oedema, pruritis and/or pain, Following ingestion: Vomiting, Irritation, Headaches and dizziness may occur, Following inhalation: Cough, pain, choking, and breathing difficulties

#### 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 (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

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

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapourair mixture. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures.

#### Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

#### 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.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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

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



#### For non-emergency personnel

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Do not breathe vapour/spray. Avoidance of ignition sources.

#### 6.2 Environmental precautions

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

#### 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.

#### Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

#### Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

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

Keep container tightly closed.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU

#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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#### Incompatible substances or mixtures

Observe hints for combined storage.

#### **Consideration of other advice:**

Ground/bond container and receiving equipment.

#### **Ventilation requirements**

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted. Use local and general ventilation.

#### 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)**

| Cou<br>ntr<br>y | Name of agent | CAS No  | Identi-<br>fier | TW<br>A<br>[pp<br>m] | TWA<br>[mg/<br>m³] | STE<br>L<br>[pp<br>m] | STEL<br>[mg/<br>m³] | Ceil<br>ing-<br>C<br>[pp<br>m] | Ceil-<br>ing-C<br>[mg/<br>m³] | Nota-<br>tion | Source                     |
|-----------------|---------------|---------|-----------------|----------------------|--------------------|-----------------------|---------------------|--------------------------------|-------------------------------|---------------|----------------------------|
| EU              | acetonitrile  | 75-05-8 | IOELV           | 40                   | 70                 |                       |                     |                                |                               | Н             | 2006/15/<br>EC             |
| IE              | acetonitrile  | 75-05-8 | OELV            | 40                   | 70                 |                       |                     |                                |                               | Н             | S.I. No.<br>619 of<br>2001 |

Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur

Ĥ STEL

Absorbed through the skin Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-TWA

minute period (unless otherwise specified) Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

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



according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV $\circledast \geq$ 99,9 %, LC-MS Grade

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| Environm      | Environmental values                      |                       |                                 |                              |  |  |  |  |  |
|---------------|---|-----------------------|---------------------------------|------------------------------|--|--|--|--|--|
| Relevant      | Relevant PNECs and other threshold levels |                       |                                 |                              |  |  |  |  |  |
| End-<br>point | Threshold<br>level                        | Organism              | Environmental com-<br>partment  | Exposure time                |  |  |  |  |  |
| PNEC          | 10 <sup>mg</sup> / <sub>l</sub>           | aquatic organisms     | freshwater                      | short-term (single instance) |  |  |  |  |  |
| PNEC          | 1 <sup>mg</sup> / <sub>l</sub>            | aquatic organisms     | marine water                    | short-term (single instance) |  |  |  |  |  |
| PNEC          | 32 <sup>mg</sup> / <sub>l</sub>           | aquatic organisms     | sewage treatment plant<br>(STP) | short-term (single instance) |  |  |  |  |  |
| PNEC          | 40,5 <sup>mg</sup> / <sub>kg</sub>        | aquatic organisms     | freshwater sediment             | short-term (single instance) |  |  |  |  |  |
| PNEC          | 4,05 <sup>mg</sup> / <sub>kg</sub>        | aquatic organisms     | marine sediment                 | short-term (single instance) |  |  |  |  |  |
| PNEC          | 2,23 <sup>mg</sup> / <sub>kg</sub>        | terrestrial organisms | soil                            | short-term (single instance) |  |  |  |  |  |

#### **Relevant PNECs of components**

| Name of sub-<br>stance        | CAS No  | End-<br>point | Threshol<br>d level                    | Organism                   | Environmental compartment       | Exposure time                   |
|-------------------------------|---------|---------------|--|----------------------------|---------------------------------|---------------------------------|
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | PNEC          | 0,56 <sup>mg</sup> / <sub>l</sub>      | aquatic organ-<br>isms     | freshwater                      | short-term (single<br>instance) |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | PNEC          | 0,056 <sup>mg</sup> / <sub>l</sub>     | aquatic organ-<br>isms     | marine water                    | short-term (single<br>instance) |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | PNEC          | 83,2 <sup>mg</sup> / <sub>l</sub>      | aquatic organ-<br>isms     | sewage treatment<br>plant (STP) | short-term (single<br>instance) |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | PNEC          | 2,36 <sup>mg</sup> / <sub>kg</sub>     | aquatic organ-<br>isms     | freshwater sedi-<br>ment        | short-term (single<br>instance) |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | PNEC          | 0,236 <sup>mg</sup> /<br><sub>kg</sub> | aquatic organ-<br>isms     | marine sediment                 | short-term (single<br>instance) |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | PNEC          | 4,7 <sup>µg</sup> / <sub>kg</sub>      | terrestrial organ-<br>isms | soil                            | short-term (single<br>instance) |

#### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

**Skin protection** 



according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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#### hand protection

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

Flame-retardant protective clothing.

#### **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).

#### **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  | faintly perceptible - like ether                 |
| Melting point/freezing point                             | -45,7 °C   |
| Boiling point or initial boiling point and boiling range | 81,65 °C at 1.013 hPa (ECHA)                     |
| Flammability   | flammable liquid in accordance with GHS criteria |
| Lower and upper explosion limit                          | 3 vol% (LEL) - 17 vol% (UEL)                     |
| Flash point  | 12,8 °C at 1.013 hPa (ECHA)                      |
| Auto-ignition temperature                                | 524 °C at 1.013 hPa (ECHA)                       |
| Decomposition temperature                                | not relevant                                     |
| pH (value)   | not determined                                   |

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

| articl | e number: <b>CP02</b>                               |  |
|--------|---|--|
|        | Kinematic viscosity                                 | 0,443 <sup>mm²</sup> / <sub>s</sub> at 20 °C                             |
|        | Dynamic viscosity                                   | 0,35 mPa s at 20 °C  |
|        | Solubility(ies)                                     |  |
|        | Water solubility                                    | miscible in any proportion   |
|        | Partition coefficient                               |  |
|        | Partition coefficient n-octanol/water (log value):  | -0,34 (pH value: ~7, 25 °C) (ECHA)                                       |
|        | Vapour pressure                                     | 94,51 hPa at 20 °C   |
|        | Density and/or relative density                     |  |
|        | Density   | 0,79 <sup>g</sup> / <sub>cm³</sub> at 20 °C (ECHA)                       |
|        | 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 classes: | There is no additional information.                                      |
|        | Other safety characteristics:                       |  |
|        | Miscibility   | completely miscible with water   |
|        | Temperature class (EU, acc. to ATEX)                | T1<br>Maximum permissible surface temperature on<br>the equipment: 450°C |

### **SECTION 10: Stability and reactivity**

#### 10.1 Reactivity

It's a reactive substance. Risk of ignition. Vapours may form explosive mixtures with air.

### If heated

Risk of ignition.

#### 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: strong oxidiser, Peroxides, Strong acid

#### 10.4 Conditions to avoid

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

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



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#### **10.5** Incompatible materials

Rubber articles

**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

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

#### Acute toxicity

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

| Acute toxicity |          |                                      |         |        |        |  |
|----------------|----------|--------------------------------------|---------|--------|--------|--|
| Exposure route | Endpoint | Value                                | Species | Method | Source |  |
| oral           | LD50     | 469 <sup>mg</sup> / <sub>kg</sub>    | mouse   |        | ECHA   |  |
| dermal         | LD50     | >2.000 <sup>mg</sup> / <sub>kg</sub> | rabbit  |        | ECHA   |  |

#### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

#### Serious eye damage/eye irritation

Causes serious eye irritation.

#### 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.

#### 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

vomiting, nausea, dizziness

#### • If in eyes

Causes serious eye irritation



according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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#### • If inhaled

cough, pain, choking, and breathing difficulties

#### • If on skin

Prolonged or repeated contact with skin or mucous membrane result in irritation symptoms such as redness, blistering, dermatitis, etc

#### • Other information

none

#### **11.2** Endocrine disrupting properties

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

#### 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) |                                    |         |        |                  |  |
|--------------------------|------------------------------------|---------|--------|------------------|--|
| Endpoint                 | Value                              | Species | Source | Exposure<br>time |  |
| LC50                     | 1.640 <sup>mg</sup> / <sub>l</sub> | fish    | ECHA   | 96 h             |  |
| ErC50                    | 9.696 <sup>mg</sup> / <sub>l</sub> | algae   | ECHA   | 72 h             |  |

#### Aquatic toxicity (acute) of components

| -                             | -       |          |                                    |                       |                  |
|-------------------------------|---------|----------|------------------------------------|-----------------------|------------------|
| Name of sub-<br>stance        | CAS No  | Endpoint | Value                              | Species               | Exposure<br>time |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | LC50     | >999 <sup>mg</sup> / <sub>l</sub>  | fish                  | 96 h             |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | EC50     | >999 <sup>mg</sup> /l              | aquatic invertebrates | 48 h             |
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | ErC50    | 237,1 <sup>mg</sup> / <sub>l</sub> | algae                 | 72 h             |

#### Aquatic toxicity (chronic)

| Endpoint | Value                               | Species        | Source | Exposure<br>time |
|----------|-------------------------------------|----------------|--------|------------------|
| EC50     | >1.000 <sup>mg</sup> / <sub>l</sub> | microorganisms | ECHA   | 30 min           |

#### Aquatic toxicity (chronic) of components

| Name of sub-<br>stance        | CAS No  | Endpoint | Value                | Species               | Exposure<br>time |
|-------------------------------|---------|----------|----------------------|-----------------------|------------------|
| Trifluoroacetic acid<br>(TFA) | 76-05-1 | EC50     | >25 <sup>mg</sup> /l | aquatic invertebrates | 21 d             |

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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#### 12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,559  $^{mg}/_{mg}$ Theoretical Oxygen Demand (with nitrification): 3,118  $^{mg}/_{mg}$ Theoretical Carbon Dioxide: 2,144  $^{mg}/_{mg}$ 

#### **Biodegradation**

The substance is readily biodegradable.

#### Process of degradability

| Process                   | Degradation rate | Time |  |  |  |  |
|---------------------------|------------------|------|--|--|--|--|
| biotic/abiotic            | 98 %             | 28 d |  |  |  |  |
| carbon dioxide generation | 70 %             | 21 d |  |  |  |  |

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

#### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

| n-octanol/water (log KOW)  |   |   | -0,34 ( | pH value: ~7, 25 °C) (ECHA) |          |
|----------------------------|---|---|---------|-----------------------------|----------|
| Bioaccumulative potentia   | Bioaccumulative potential of components |   |         |                             |          |
| Name of substance          | CAS No                                  | В | CF      | 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

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

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.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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#### Sewage disposal-relevant information

Do not empty into drains.

#### Waste treatment of containers/packagings

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

#### 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.

#### Properties of waste which render it hazardous

- **HP3** flammable
- **HP 4** irritant skin irritation and eye damage
- HP 6 acute toxicity

#### 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.

### **SECTION 14: Transport information**

#### 14.1 UN number or ID number

| 14.5 | Environmental hazards      | non-environmentally hazardous acc. to the dan-<br>gerous goods regulations |
|------|----------------------------|--|
|      | ICAO-TI                    | II   |
|      | IMDG-Code                  | II   |
|      | ADRRID                     | II   |
| 14.4 | Packing group              |  |
|      | ICAO-TI                    | 3  |
|      | IMDG-Code                  | 3  |
|      | ADRRID                     | 3  |
| 14.3 | Transport hazard class(es) |  |
|      | ICAO-TI                    | Acetonitrile   |
|      | IMDG-Code                  | ACETONITRILE   |
|      | ADRRID                     | ACETONITRILE   |
| 14.2 | UN proper shipping name    |  |
|      | ICAO-TI                    | UN 1648  |
|      | IMDG-Code                  | UN 1648  |
|      | ADRRID                     | UN 1648  |
| 14.1 |                            |  |

#### 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.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV $\circledast \geq \! 99,9$ %, LC-MS Grade

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| 14.8 | Information for each of the UN Model Regulations  |   |  |  |  |
|------|---|---|--|--|--|
|      | Agreement concerning the International Carria<br>information  | ge of Dangerous Goods by Road (ADR)Additional |  |  |  |
|      | Proper shipping name  | ACETONITRILE                                  |  |  |  |
|      | Particulars in the transport document   | UN1648, ACETONITRILE, 3, II, (D/E)            |  |  |  |
|      | Classification code   | F1  |  |  |  |
|      | Danger label(s)   | 3   |  |  |  |
|      |   |   |  |  |  |
|      | Excepted quantities (EQ)  | E2  |  |  |  |
|      | Limited quantities (LQ)   | 1 L   |  |  |  |
|      | Transport category (TC)   | 2   |  |  |  |
|      | Tunnel restriction code (TRC)   | D/E   |  |  |  |
|      | Hazard identification No  | 33  |  |  |  |
|      | Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additiona information |   |  |  |  |
|      | Classification code   | F1  |  |  |  |
|      | Danger label(s)   | 3   |  |  |  |
|      |   |   |  |  |  |
|      | Excepted quantities (EQ)  | E2  |  |  |  |
|      | Limited quantities (LQ)   | 1 L   |  |  |  |
|      | Transport category (TC)   | 2   |  |  |  |
|      | Hazard identification No  | 33  |  |  |  |
|      | International Maritime Dangerous Goods Code   | (IMDG) - Additional information               |  |  |  |
|      | Proper shipping name  | ACETONITRILE                                  |  |  |  |
|      | Particulars in the shipper's declaration  | UN1648, ACETONITRILE, 3, II, 12,8°C c.c.      |  |  |  |
|      | Marine pollutant  | -   |  |  |  |
|      | Danger label(s)   | 3   |  |  |  |
|      |   |   |  |  |  |
|      | Excepted quantities (EQ)  | E2  |  |  |  |
|      | Limited quantities (LQ)   | 1 L   |  |  |  |
|      | EmS   | F-E, S-D                                      |  |  |  |
|      | Stowage category  | В   |  |  |  |

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



#### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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| International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information |                             |  |  |
|--|-----------------------------|--|--|
| Proper shipping name   | Acetonitrile                |  |  |
| Particulars in the shipper's declaration   | UN1648, Acetonitrile, 3, II |  |  |
| Danger label(s)  | 3                           |  |  |
| Excepted quantities (EQ)   | E2                          |  |  |
| Limited quantities (LQ)  | 1 L                         |  |  |
|  |                             |  |  |

### **SECTION 15: Regulatory information**

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

#### **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 |
| Acetonitrile with 0,1 % Trifluoroacetic acid               | this product meets the criteria for<br>classification in accordance with Reg-<br>ulation No 1272/2008/EC |        | R3          | 3  |
| Acetonitrile with 0,1 % Trifluoroacetic acid               | flammable / pyrophoric   |        | R40         | 40 |
| Acetonitrile with 0,1 % Trifluoroacetic acid               | substances in tattoo inks and perman-<br>ent make-up   |        | R75         | 75 |

#### Legend R3

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,

or both. if they

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.
 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

(CEN). 5. Without prejudice to the implementation of other Union provisions relating to the classification, labelling and pack-aging of substances and mixtures, suppliers shall ensure, before the placing on the market, that the following requirements are met:

ments are met: (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"; (b) grill lighter fluids, 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.';

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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#### Legend R40

- 1. Shall not be used, as substance or as mixtures in aerosol dispensers where these aerosol dispensers are intended for supply to the general public for entertainment and decorative purposes such as the following: metallic glitter intended mainly for decoration,
- artificial snow and frost,
- 'whoopee' cushions,

- silly string aerosols,
  imitation excrement,
  horns for parties,
  decorative flakes and foams,
- artificial cobwebs,
- stink bombs.

Without prejudice to the application of other Community provisions on the classification, packaging and labelling of substances, suppliers shall ensure before the placing on the market that the packaging of aerosol dispensers referred to above is marked visibly, legibly and indelibly with: 'For professional users only'.

- 3. By way of derogation, paragraphs 1 and 2 shall not apply to the aerosol dispensers referred to Article 8 (1a) of Council Directive 75/324/EEC (2).

4. The aerosol dispensers referred to in paragraphs 1 and 2 shall not be placed on the market unless they conform to the requirements indicated.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV® ≥99,9 %, LC-MS Grade

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8. Mixtures that do not contain the statement "Mixture for use in tattoos or permanent make-up" shall not be used for tattooing purposes.

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV $\circledast \geq \!\! 99,9$ %, LC-MS Grade

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#### Legend

9. This entry does not apply to substances that are gases at temperature of 20 °C and pressure of 101,3 kPa, or generate a vapour pressure of more than 300 kPa at temperature of 50 °C, with the exception of formaldehyde (CAS No 50-00-0, EC No 200-001-8).

10. This entry does not apply to the placing on the market of a mixture for use for tattooing purposes, or to the use of a mixture for tattooing purposes, when placed on the market exclusively as a medical device or an accessory to a medical device, within the meaning of Regulation (EU) 2017/745, or when used exclusively as a medical device or an accessory to a medical device, within the same meaning. Where the placing on the market or use may not be exclusively as a medical device or an accessory to a medical device or an accessory to a medical device, within the same meaning. Where the placing on the market or use may not be exclusively as a medical device or an accessory to a medical device, the requirements of Regulation (EU) 2017/745 and of this Regulation shall apply cumulatively.

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

Not listed.

#### **Seveso Directive**

| 2012/ | 18/EU (Seveso III)                    |   |        |       |
|-------|---------------------------------------|---|--------|-------|
| No    | Dangerous substance/hazard categories | Qualifying quantity (tonnes) for the ap-<br>plication of lower and upper-tier re-<br>quirements |        | Notes |
| P5c   | flammable liquids (cat. 2, 3)         | 5.000   | 50.000 | 51)   |

#### Notation

51) Flammable liquids, categories 2 or 3 not covered by P5a and P5b

#### **Deco-Paint Directive**

| VOC content | 100 %               |
|-------------|---------------------|
| VOC content | 790 <sup>g</sup> /l |

#### Industrial Emissions Directive (IED)

| VOC content | 100 %                           |
|-------------|---------------------------------|
| VOC content | 790 <sup>g</sup> / <sub>l</sub> |

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

not listed

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

not listed

#### Water Framework Directive (WFD)

not listed

#### Regulation on the marketing and use of explosives precursors

not listed

#### **Regulation on drug precursors**

not listed

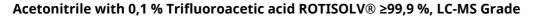
#### **Regulation on substances that deplete the ozone layer (ODS)**

not listed

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

not listed

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



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# Regulation on persistent organic pollutants (POP)

not 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          |
| JP      | CSCL-ENCS  | substance is listed          |
| KR      | KECI       | substance is listed          |
| MX      | INSQ       | substance is listed          |
| NZ      | NZIoC      | substance is listed          |
| PH      | PICCS      | substance is listed          |
| TR      | CICR       | substance is listed          |
| TW      | TCSI       | substance is listed          |
| US      | TSCA       | substance is listed (ACTIVE) |
| VN      | NCI        | substance is listed          |

#### Legend

| Australian Inventory of Industrial Chemicals                            |
|---|
| Chemical Inventory and Control Regulation                               |
| 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                               |
| Korea Existing Chemicals Inventory                                      |
| National Chemical Inventory   |
| New Zealand Inventory of Chemicals                                      |
| Philippine Inventory of Chemicals and Chemical Substances (PICCS)       |
| REACH registered substances   |
| Taiwan Chemical Substance Inventory                                     |
| Toxic Substance Control Act   |
|   |

#### 15.2 Chemical safety assessment

According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.



according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV $\circledast \geq \!\! 99,9$ %, LC-MS Grade

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### **SECTION 16: Other information**

#### Indication of changes (revised safety data sheet)

| Section | Former entry (text/value)  | Actual entry (text/value)   | Safety-<br>relev-<br>ant |
|---------|--|---|--------------------------|
| 2.3     |  | Endocrine disrupting properties:<br>Does not contain an endocrine disruptor (ED) at<br>a concentration of ≥ 0,1%.   | yes                      |
| 14.8    |  | Regulations concerning the International Car-<br>riage of Dangerous Goods by Rail (RID)Addition-<br>al information  | yes                      |
| 14.8    |  | Classification code:<br>F1  | yes                      |
| 14.8    |  | Danger label(s):<br>3   | yes                      |
| 14.8    |  | Danger label(s):<br>change in the listing (table)   | yes                      |
| 14.8    |  | Excepted quantities (EQ):<br>E2   | yes                      |
| 14.8    |  | Limited quantities (LQ):<br>1 L   | yes                      |
| 14.8    |  | Transport category (TC):<br>2   | yes                      |
| 14.8    |  | Hazard identification No:<br>33   | yes                      |
| 15.1    | VOC content:<br>100 %<br>, 790 <sup>g</sup> / <sub>l</sub>   | VOC content:<br>100 %   | yes                      |
| 15.1    |  | VOC content:<br>790 <sup>g</sup> / <sub>l</sub>   | yes                      |
| 15.1    |  | National inventories:<br>change in the listing (table)  | yes                      |
| 15.2    | Chemical Safety Assessment:<br>No Chemical Safety Assessment has been car-<br>ried out for this substance. | Chemical safety assessment:<br>According to REACH, Article 14 (1) a chemical<br>safety assessment has been carried out for this<br>substance or components of this mixture when<br>the substance has been registered in quantities<br>of 10 tonnes or more per year per registrant. | yes                      |

#### Abbreviations and acronyms

| Abbr.      | Descriptions of used abbreviations  |
|------------|---|
| 2006/15/EC | Commission Directive establishing a second list of indicative occupational exposure limit values in imple-<br>mentation of Council Directive 98/24/EC and amending Directives 91/322/EEC and 2000/39/EC |
| ADR        | Accord relatif au transport international des marchandises dangereuses par route (Agreement concern-<br>ing the International Carriage of Dangerous Goods by Road)                                      |
| 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)  |

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV $\circledast \geq \! 99,9$ %, LC-MS Grade

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| Abbr.     | Descriptions of used abbreviations  |
|-----------|---|
| Ceiling-C | Ceiling value   |
| 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 ident fier of substances commercially available within the EU (European Union) |
| 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 Na<br>tions   |
| 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  |
| IOELV     | Indicative occupational exposure limit value  |
| LC50      | Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50<br>lethality during a specified time interval                                |
| LD50      | Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during specified time interval  |
| LEL       | Lower explosion limit (LEL)   |
| log KOW   | n-Octanol/water   |
| NLP       | No-Longer Polymer   |
| PBT       | Persistent, Bioaccumulative and Toxic   |
| PNEC      | Predicted No-Effect Concentration   |
| ppm       | Parts per million   |
| REACH     | Registration, Evaluation, Authorisation and Restriction of Chemicals  |
| RID       | Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regula-<br>tions concerning the International carriage of Dangerous goods by Rail)      |

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



### Acetonitrile with 0,1 % Trifluoroacetic acid ROTISOLV $\circledast \geq \!\! 99,9$ %, LC-MS Grade

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| Abbr.                   | Descriptions of used abbreviations                                    |
|-------------------------|---|
| S.I. No. 619 of<br>2001 | Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001 |
| STEL                    | Short-term exposure limit   |
| SVHC                    | Substance of Very High Concern  |
| TWA                     | Time-weighted average   |
| UEL                     | Upper explosion limit (UEL)   |
| 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.

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                                |
|------|-------------------------------------|
| H225 | Highly flammable liquid and vapour. |
| H302 | Harmful if swallowed.               |
| H312 | Harmful in contact with skin.       |
| H319 | Causes serious eye irritation.      |
| 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.