

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 20.02.2018

Version 9.10

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

### 1.1 Product identifier

Catalogue No. 808259

Product name 2,2,2-Trifluoroethanol for synthesis

REACH Registration Number A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. 75-89-8

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

Identified uses Chemical for synthesis  
For additional information on uses please refer to the Merck Chemicals portal ([www.merckgroup.com](http://www.merckgroup.com)).

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

Company Merck KGaA \* 64271 Darmstadt \* Germany \* Phone:+49 6151 72-0

Responsible Department LS-QHC \* e-mail: [prodsafe@merckgroup.com](mailto:prodsafe@merckgroup.com)

1.4 Emergency telephone number **Please contact the regional company representation in your country.**

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## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 3, H226

Acute toxicity, Category 3, Oral, H301

Acute toxicity, Category 3, Inhalation, H331

Serious eye damage, Category 1, H318

Reproductive toxicity, Category 1B, H360F

Specific target organ toxicity - repeated exposure, Category 2, Blood, H373

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 2.2 Label elements

#### Labelling (REGULATION (EC) No 1272/2008)

##### *Hazard pictograms*



##### *Signal word*

Danger

##### *Hazard statements*

H360F May damage fertility.

H226 Flammable liquid and vapour.

H301 + H331 Toxic if swallowed or if inhaled.

H318 Causes serious eye damage.

H373 May cause damage to organs (Blood) through prolonged or repeated exposure.

##### *Precautionary statements*

Prevention

P201 Obtain special instructions before use.

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P210 Keep away from heat.

P280 Wear eye protection.

Response

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Restricted to professional users.

**Reduced labelling (≤125 ml)**

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H360F May damage fertility.

H301 + H331 Toxic if swallowed or if inhaled.

H318 Causes serious eye damage.

*Precautionary statements*

P201 Obtain special instructions before use.

P280 Wear eye protection.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

*CAS-No.* 75-89-8

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

|            |                                    |   |
|------------|------------------------------------|---|
| Formula    | CF <sub>3</sub> CH <sub>2</sub> OH | C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O (Hill) |
| EC-No.     | 200-913-6                          |   |
| Molar mass | 100,04 g/mol                       |   |

### Hazardous components (REGULATION (EC) No 1272/2008)

*Chemical name (Concentration)*

| CAS-No. | Registration number | Classification |
|---------|---------------------|----------------|
|---------|---------------------|----------------|

2,2,2-trifluoroethanol (<= 100 % )

75-89-8 \*)

Flammable liquid, Category 3, H226

Acute toxicity, Category 3, H301

Acute toxicity, Category 3, H331

Serious eye damage, Category 1, H318

Reproductive toxicity, Category 1B, H360F

Specific target organ toxicity - repeated exposure, Category 2,  
H373

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 3.2 Mixture

Not applicable

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

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## *General advice*

First aider needs to protect himself.

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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

Cough, Shortness of breath, Diarrhoea, Nausea, Vomiting, ataxia (impaired locomotor coordination), Tremors

Irritation and corrosion

Risk of serious damage to eyes.

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

No information available.

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## **SECTION 5. Firefighting measures**

### **5.1 Extinguishing media**

#### *Suitable extinguishing media*

Water, Foam, Carbon dioxide (CO<sub>2</sub>), Dry powder

#### *Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

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

Combustible.

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Vapours are heavier than air and may spread along floors.  
Forms explosive mixtures with air at elevated temperatures.  
Development of hazardous combustion gases or vapours possible in the event of fire.  
Fire may cause evolution of:  
Hydrogen fluoride

## 5.3 Advice for firefighters

*Special protective equipment for firefighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

*Further information*

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6. Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

### 6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

### 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

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Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

#### *Advice on safe handling*

Observe label precautions.

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### *Advice on protection against fire and explosion*

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### *Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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

#### *Storage conditions*

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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## SECTION 8. Exposure controls/personal protection

### 8.1 Control parameters

### 8.2 Exposure controls

#### Engineering measures

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Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

## Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

### *Eye/face protection*

Tightly fitting safety goggles

### *Hand protection*

full contact:

|                     |                 |
|---------------------|-----------------|
| Glove material:     | polychloroprene |
| Glove thickness:    | 0,65 mm         |
| Break through time: | > 480 min       |

splash contact:

|                     |                |
|---------------------|----------------|
| Glove material:     | Nitrile rubber |
| Glove thickness:    | 0,40 mm        |
| Break through time: | > 30 min       |

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 720 Camapren® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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

### *Other protective equipment*

Flame retardant antistatic protective clothing.



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## *Respiratory protection*

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

## **Environmental exposure controls**

Do not let product enter drains.

Risk of explosion.

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## **SECTION 9. Physical and chemical properties**

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

|                             |                           |
|-----------------------------|---------------------------|
| Form                        | liquid                    |
| Colour                      | colourless                |
| Odour                       | characteristic            |
| Odour Threshold             | No information available. |
| pH                          | neutral                   |
| Melting point               | -43,5 °C                  |
| Boiling point/boiling range | 73,6 °C<br>at 1.013 hPa   |
| Flash point                 | 30 °C                     |
| Evaporation rate            | No information available. |

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|  |   |
|--|---|
| Flammability (solid, gas)              | No information available.   |
| Lower explosion limit                  | 8,4 %(V)  |
| Upper explosion limit                  | 28,8 %(V)   |
| Vapour pressure                        | 70,9 hPa<br>at 20 °C<br>Method: OECD Test Guideline 104                               |
| Relative vapour density                | 3,5   |
| Density                                | 1,38 g/cm <sup>3</sup><br>at 25 °C<br>Method: OECD Test Guideline 109                 |
| Relative density                       | No information available.   |
| Water solubility                       | at 20 °C<br>soluble   |
| Partition coefficient: n-octanol/water | log Pow: < 0,3 (25 °C)<br>OECD Test Guideline 117<br>Bioaccumulation is not expected. |
| Auto-ignition temperature              | No information available.   |
| Decomposition temperature              | 315 °C  |
| Viscosity, dynamic                     | 1,722 mPa.s<br>at 25 °C<br>Method: OECD Test Guideline 114                            |
| Explosive properties                   | Not classified as explosive.  |

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Oxidizing properties none

## 9.2 Other data

none

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## SECTION 10. Stability and reactivity

### 10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, strong alkalis

### 10.4 Conditions to avoid

Exposure to moisture

Heating.

### 10.5 Incompatible materials

no information available

### 10.6 Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 Rat: 153 mg/kg

OECD Test Guideline 401

Symptoms: Irritation of mucous membranes, Diarrhoea, Nausea, Vomiting

#### *Acute inhalation toxicity*

LC50 Rat: 3,25 mg/l/784 ppm; 4 h ; vapour

OECD Test Guideline 403

Symptoms: Possible damages:, Irritation symptoms in the respiratory tract.

#### *Acute dermal toxicity*

LD50 Rat: > 2.000 mg/kg

OECD Test Guideline 402

#### *Skin irritation*

Rabbit

Result: No skin irritation

OECD Test Guideline 404

#### *Eye irritation*

Rabbit

Result: Irreversible effects on the eye

OECD Test Guideline 405

Causes serious eye damage.

Risk of serious damage to eyes.

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## *Sensitisation*

Local lymph node assay (LLNA) Mouse

Result: negative

Method: OECD Test Guideline 429

## *Germ cell mutagenicity*

### *Genotoxicity in vitro*

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Mutagenicity (mammal cell test): chromosome aberration.

Chinese hamster ovary cells

Result: negative

Method: OECD Test Guideline 473

In vitro mammalian cell gene mutation test

Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 476

## *Carcinogenicity*

This information is not available.

## *Reproductive toxicity*

This information is not available.

## *Teratogenicity*

This information is not available.

## *CMR effects*

Reproductive toxicity:

May damage fertility.

## *Specific target organ toxicity - single exposure*

This information is not available.

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### *Specific target organ toxicity - repeated exposure*

May cause damage to organs through prolonged or repeated exposure.

Target Organs: Blood

### *Aspiration hazard*

This information is not available.

## 11.2 Further information

After absorption:

Systemic effects:

ataxia (impaired locomotor coordination), Tremors

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

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## SECTION 12. Ecological information

### 12.1 Toxicity

#### *Toxicity to daphnia and other aquatic invertebrates*

semi-static test EC50 Daphnia magna (Water flea): > 1.000 mg/l; 48 h

OECD Test Guideline 202

#### *Toxicity to algae*

static test ErC50 Pseudokirchneriella subcapitata (green algae): > 974 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

#### *Toxicity to bacteria*

static test EC50 activated sludge: > 1.000 mg/l; 3 h

OECD Test Guideline 209

### 12.2 Persistence and degradability

#### *Biodegradability*

0 %; 28 d; aerobic

OECD Test Guideline 310

Not readily biodegradable.

### 12.3 Bioaccumulative potential

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*Partition coefficient: n-octanol/water*

log Pow: < 0,3 (25 °C)

OECD Test Guideline 117

Bioaccumulation is not expected.

## 12.4 Mobility in soil

No information available.

## 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

## 12.6 Other adverse effects

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14. Transport information

### Land transport (ADR/RID)

|                                   |  |
|-----------------------------------|--|
| 14.1 UN number                    | UN 1992  |
| 14.2 Proper shipping name         | FLAMMABLE LIQUID, TOXIC, N.O.S. (2,2,2-TRIFLUOROETHANOL) |
| 14.3 Class                        | 3 (6.1)  |
| 14.4 Packing group                | III  |
| 14.5 Environmentally hazardous    | --   |
| 14.6 Special precautions for user | yes  |
| Tunnel restriction code           | D/E  |

### Inland waterway transport (ADN)

Not relevant

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## Air transport (IATA)

14.1 UN number UN 1992  
14.2 Proper shipping name FLAMMABLE LIQUID, TOXIC, N.O.S. (2,2,2-TRIFLUOROETHANOL)  
14.3 Class 3 (6.1)  
14.4 Packing group III  
14.5 Environmentally hazardous --  
14.6 Special precautions for user no

## Sea transport (IMDG)

14.1 UN number UN 1992  
14.2 Proper shipping name FLAMMABLE LIQUID, TOXIC, N.O.S. (2,2,2-TRIFLUOROETHANOL)  
14.3 Class 3 (6.1)  
14.4 Packing group III  
14.5 Environmentally hazardous --  
14.6 Special precautions for user yes  
EmS F-E S-D

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code  
Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

Major Accident Hazard SEVESO III  
Legislation ACUTE TOXIC  
H2  
Quantity 1: 50 t  
Quantity 2: 200 t



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SEVESO III  
FLAMMABLE LIQUIDS  
P5c  
Quantity 1: 5.000 t  
Quantity 2: 50.000 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

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

### *National legislation*

Storage class 3

## 15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

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## SECTION 16. Other information

### Full text of H-Statements referred to under sections 2 and 3.

|       |  |
|-------|--|
| H226  | Flammable liquid and vapour.                                       |
| H301  | Toxic if swallowed.  |
| H318  | Causes serious eye damage.   |
| H331  | Toxic if inhaled.  |
| H360F | May damage fertility.  |
| H373  | May cause damage to organs through prolonged or repeated exposure. |

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

#### *Hazard pictograms*



#### *Signal word*

Danger

#### *Hazard statements*

H226 Flammable liquid and vapour.  
H301 + H331 Toxic if swallowed or if inhaled.  
H318 Causes serious eye damage.  
H360 May damage fertility or the unborn child.  
H373 May cause damage to organs (Blood) through prolonged or repeated exposure.

#### *Precautionary statements*

Prevention

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|               |                                      |
|---------------|--------------------------------------|
| Catalogue No. | 808259                               |
| Product name  | 2,2,2-Trifluoroethanol for synthesis |

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P201 Obtain special instructions before use.

P210 Keep away from heat.

P280 Wear eye protection.

Response

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Further information

Restricted to professional users.

## Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

## Regional representation

This information is given on the authorised Safety Data Sheet for your country.

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*