

Creation Date 10-Sep-2009

Revision Date 06-Oct-2023

Revision Number 5

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

Product Description: Ethyl 4,4,4-trifluoro-2-butynoate  
Cat No. : 399320000; 399320050  
CAS No 79424-03-6  
Molecular Formula C6 H5 F3 O2

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

Recommended Use Laboratory chemicals.  
Uses advised against No Information available

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

#### Company

**UK entity/business name**  
Fisher Scientific UK  
Bishop Meadow Road,  
Loughborough, Leicestershire LE11 5RG, United Kingdom

**EU entity/business name**  
Thermo Fisher Scientific  
Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

### 1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

##### Physical hazards

Flammable liquids Category 2 (H225)

##### Health hazards

Acute oral toxicity Category 4 (H302)  
Acute dermal toxicity Category 4 (H312)

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Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Specific target organ toxicity - (single exposure)

Category 2 (H315)  
Category 2 (H319)  
Category 3 (H335)

## **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



Signal Word

Danger

## **Hazard Statements**

H225 - Highly flammable liquid and vapor  
H315 - Causes skin irritation  
H335 - May cause respiratory irritation  
H319 - Causes serious eye irritation  
H302 + H312 - Harmful if swallowed or in contact with skin

## **Precautionary Statements**

P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P240 - Ground and bond container and receiving equipment  
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

## **2.3. Other hazards**

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### **3.1. Substances**

| Component                         | CAS No     | EC No | Weight % | CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567                       |
|-----------------------------------|------------|-------|----------|---------------------------------------------------------------------------------------------------------------|
| Ethyl 4,4,4-trifluoro-2-butynoate | 79424-03-6 |       | >95      | Flam. Liq. 2 (H225)<br>STOT SE 3 (H335)<br>Skin Irrit. 2 (H315)<br>Eye Irrit. 2 (H319)<br>Acute Tox. 4 (H302) |

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|  |  |  |  |                     |
|--|--|--|--|---------------------|
|  |  |  |  | Acute Tox. 4 (H312) |
|--|--|--|--|---------------------|

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

|                                           |                                                                                                                                                                                                                                                                                                                                |
|-------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Eye Contact</b>                        | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.                                                                                                                                                                                              |
| <b>Skin Contact</b>                       | Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.                                                                                                                                                                                                                    |
| <b>Ingestion</b>                          | Do NOT induce vomiting. Call a physician or poison control center immediately.                                                                                                                                                                                                                                                 |
| <b>Inhalation</b>                         | Remove to fresh air. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required. If not breathing, give artificial respiration. |
| <b>Self-Protection of the First Aider</b> | Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.                                                                                                                                                                               |

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

Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

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

|                           |                        |
|---------------------------|------------------------|
| <b>Notes to Physician</b> | Treat symptomatically. |
|---------------------------|------------------------|

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### Suitable Extinguishing Media

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

#### Extinguishing media which must not be used for safety reasons

No information available.

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

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

#### Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

### 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full

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protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

### 6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

### 6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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

Keep containers tightly closed in a dry, cool and well-ventilated place. Flammables area. Keep away from heat, sparks and flame.

Technical Rules for Hazardous Substances (TRGS) 510      Class 3  
Storage Class (LGK) (Germany)

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

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## Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. Ensure adequate ventilation, especially in confined areas. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

### Personal protective equipment

#### Eye Protection

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

| Glove material                                      | Breakthrough time                    | Glove thickness | EU standard | Glove comments        |
|-----------------------------------------------------|--------------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber<br>Neoprene<br>Natural rubber<br>PVC | See manufacturers<br>recommendations | -               | EN 374      | (minimum requirement) |

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

#### Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

#### Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

#### Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

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**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

|                                         |                               |                                          |
|-----------------------------------------|-------------------------------|------------------------------------------|
| Physical State                          | Liquid                        |                                          |
| Appearance                              |                               |                                          |
| Odor                                    | No information available      |                                          |
| Odor Threshold                          | No data available             |                                          |
| Melting Point/Range                     | No data available             |                                          |
| Softening Point                         | No data available             |                                          |
| Boiling Point/Range                     | 96 - 98 °C / 204.8 - 208.4 °F | @ 760 mmHg                               |
| Flammability (liquid)                   | Highly flammable              | On basis of test data                    |
| Flammability (solid,gas)                | Not applicable                | Liquid                                   |
| Explosion Limits                        | No data available             |                                          |
| Flash Point                             | 6 °C / 42.8 °F                | <b>Method -</b> No information available |
| Autoignition Temperature                | No data available             |                                          |
| Decomposition Temperature               | No data available             |                                          |
| pH                                      | No information available      |                                          |
| Viscosity                               | No data available             |                                          |
| Water Solubility                        | No information available      |                                          |
| Solubility in other solvents            | No information available      |                                          |
| Partition Coefficient (n-octanol/water) |                               |                                          |
| Vapor Pressure                          | No data available             |                                          |
| Density / Specific Gravity              | 1.62                          |                                          |
| Bulk Density                            | Not applicable                | Liquid                                   |
| Vapor Density                           | No data available             | (Air = 1.0)                              |
| Particle characteristics                | Not applicable (liquid)       |                                          |

### 9.2. Other information

|                      |                                             |
|----------------------|---------------------------------------------|
| Molecular Formula    | C6 H5 F3 O2                                 |
| Molecular Weight     | 166.10                                      |
| Explosive Properties | Vapors may form explosive mixtures with air |

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

|                          |                                          |
|--------------------------|------------------------------------------|
| Hazardous Polymerization | Hazardous polymerization does not occur. |
| Hazardous Reactions      | None under normal processing.            |

### 10.4. Conditions to avoid

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and

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sources of ignition.

## 10.5. Incompatible materials

Strong oxidizing agents.

## 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

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

#### Product Information

##### (a) acute toxicity;

|            |                   |
|------------|-------------------|
| Oral       | Category 4        |
| Dermal     | Category 4        |
| Inhalation | No data available |

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

##### (d) respiratory or skin sensitization;

|             |                   |
|-------------|-------------------|
| Respiratory | No data available |
| Skin        | No data available |

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

**Other Adverse Effects** The toxicological properties have not been fully investigated.

**Symptoms / effects, both acute and delayed** Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

### 11.2. Information on other hazards

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**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

**Ecotoxicity effects** Do not empty into drains.

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB assessment No data available for assessment.

### 12.6. Endocrine disrupting properties

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

### 12.7. Other adverse effects

**Persistent Organic Pollutant** This product does not contain any known or suspected substance  
**Ozone Depletion Potential** This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

**Waste from Residues/Unused Products** Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging** Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

**European Waste Catalogue (EWC)** According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

**Other Information** Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

ACR39932

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**14.1. UN number** UN3272  
**14.2. UN proper shipping name** Esters, n.o.s  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** II

## ADR

**14.1. UN number** UN3272  
**14.2. UN proper shipping name** Esters, n.o.s  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** II

## IATA

**14.1. UN number** UN3272  
**14.2. UN proper shipping name** Esters, n.o.s  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** II

**14.5. Environmental hazards** No hazards identified  
**14.6. Special precautions for user** No special precautions required.  
**14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component                         | CAS No     | EINECS | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|-----------------------------------|------------|--------|--------|-----|-------|------|------|------|------|
| Ethyl 4,4,4-trifluoro-2-butynoate | 79424-03-6 | -      | -      | -   | -     | X    | -    | -    | -    |

| Component                         | CAS No     | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|-----------------------------------|------------|------|-----------------------------------------------|-----|------|------|-------|-------|
| Ethyl 4,4,4-trifluoro-2-butynoate | 79424-03-6 | -    | -                                             | -   | -    | -    | -     | -     |

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH Not applicable

| Component                         | CAS No     | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|-----------------------------------|------------|---------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| Ethyl 4,4,4-trifluoro-2-butynoate | 79424-03-6 | -                                                                   | -                                                                             | -                                                                                                     |

#### Seveso III Directive (2012/18/EC)

| Component | CAS No | Seveso III Directive (2012/18/EC) - | Seveso III Directive (2012/18/EC) - |
|-----------|--------|-------------------------------------|-------------------------------------|
|-----------|--------|-------------------------------------|-------------------------------------|

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|                                   |            | Qualifying Quantities for Major Accident Notification | Qualifying Quantities for Safety Report Requirements |
|-----------------------------------|------------|-------------------------------------------------------|------------------------------------------------------|
| Ethyl 4,4,4-trifluoro-2-butynoate | 79424-03-6 | Not applicable                                        | Not applicable                                       |

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

See table for values

| Component                                             | OECD PFAS | US (EPA) PFAS | EU (ECHA) PFAS | UK (HSE) PFAS | Chemsec PFAS (Sin List) |
|-------------------------------------------------------|-----------|---------------|----------------|---------------|-------------------------|
| Ethyl 4,4,4-trifluoro-2-butynoate (CAS #: 79424-03-6) | -         | -             | Listed         | Listed        | -                       |

## PFAS Legend

Listed = Meets the PFAS definition of the named authority

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** Water endangering class = 3 (self classification)

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

H225 - Highly flammable liquid and vapor

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

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**WEL** - Workplace Exposure Limit  
**ACGIH** - American Conference of Governmental Industrial Hygienists  
**DNEL** - Derived No Effect Level  
**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average  
**IARC** - International Agency for Research on Cancer  
Predicted No Effect Concentration (PNEC)  
**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code  
**OECD** - Organisation for Economic Co-operation and Development  
**BCF** - Bioconcentration factor

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association  
**MARPOL** - International Convention for the Prevention of Pollution from Ships  
**ATE** - Acute Toxicity Estimate  
**VOC** - (Volatile Organic Compound)

## Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>  
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

## Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

|                         |                 |
|-------------------------|-----------------|
| <b>Creation Date</b>    | 10-Sep-2009     |
| <b>Revision Date</b>    | 06-Oct-2023     |
| <b>Revision Summary</b> | Not applicable. |

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**