

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 7.3

Revision Date 04.05.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

### 1.1 Product identifiers

Product name : Acetonitrile, for UHPLC, for mass spectrometry

Product Number : 900667  
Brand : Sigma-Aldrich  
Index-No. : 608-001-00-3  
REACH No. : 01-2119471307-38-XXXX  
CAS-No. : 75-05-8

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

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### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

Flammable liquids (Category 2), H225  
Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 4), H332  
Acute toxicity, Dermal (Category 4), H312  
Eye irritation (Category 2), H319

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

## 2.2 Label elements

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

Pictogram

|                                |                                                                                                                                  |
|--------------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| Signal Word                    | Danger                                                                                                                           |
| Hazard statement(s)            |                                                                                                                                  |
| H225                           | Highly flammable liquid and vapor.                                                                                               |
| H302 + H312 + H332             | Harmful if swallowed, in contact with skin or if inhaled.                                                                        |
| H319                           | Causes serious eye irritation.                                                                                                   |
| Precautionary statement(s)     |                                                                                                                                  |
| 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.                                                    |
| P301 + P312                    | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.                                                                   |
| P303 + P361 + P353             | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.                                     |
| P304 + P340 + P312             | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.      |
| P305 + P351 + P338             | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| Supplemental Hazard Statements | none                                                                                                                             |

### Reduced Labeling (<= 125 ml)

Pictogram

|                                |        |
|--------------------------------|--------|
| Signal Word                    | Danger |
| Hazard statement(s)            | none   |
| Precautionary statement(s)     | none   |
| Supplemental Hazard Statements | none   |

## 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : ACN

## Methyl cyanide

Formula : C<sub>2</sub>H<sub>3</sub>N  
Molecular weight : 41,05 g/mol  
CAS-No. : 75-05-8  
EC-No. : 200-835-2  
Index-No. : 608-001-00-3

| Component           |              | Classification              | Concentration |
|---------------------|--------------|-----------------------------|---------------|
| <b>Acetonitrile</b> |              |                             |               |
| CAS-No.             | 75-05-8      | Flam. Liq. 2; Acute Tox. 4; | <= 100 %      |
| EC-No.              | 200-835-2    | Eye Irrit. 2; H225, H302,   |               |
| Index-No.           | 608-001-00-3 | H332, H312, H319            |               |

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

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

#### In case of skin contact

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

#### In case of eye contact

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

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

## 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**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

**5.3 Advice 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.

**5.4 Further information**

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/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 vapors, 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. For personal protection 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 with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

**6.4 Reference to other sections**

For disposal see section 13.

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**SECTION 7: Handling and storage****7.1 Precautions for safe handling****Advice on safe handling**

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.

For precautions see section 2.2.

## 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.

Handle and store under inert gas.

### Storage class

Storage class (TRGS 510): 3: Flammable liquids

## 7.3 Specific end use(s)

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

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

##### Derived No Effect Level (DNEL)

| Application Area | Routes of exposure | Health effect                                       | Value                 |
|------------------|--------------------|-----------------------------------------------------|-----------------------|
| Workers          | Inhalation         | Acute local effects, Acute systemic effects         | 68 mg/m <sup>3</sup>  |
| Workers          | Skin contact       | Long-term systemic effects                          | 32,2mg/kg BW/d        |
| Workers          | Inhalation         | Long-term local effects, Long-term systemic effects | 68 mg/m <sup>3</sup>  |
| Consumers        | Inhalation         | Acute local effects                                 | 220 mg/m <sup>3</sup> |
| Consumers        | Inhalation         | Acute systemic effects                              | 22 mg/m <sup>3</sup>  |
| Consumers        | Inhalation         | Long-term systemic effects                          | 4,8 mg/m <sup>3</sup> |

##### Predicted No Effect Concentration (PNEC)

| Compartment                   | Value      |
|-------------------------------|------------|
| Water                         | 10 mg/l    |
| Soil                          | 2,41 mg/kg |
| Sea water                     | 1 mg/l     |
| Fresh water                   | 10 mg/l    |
| Fresh water sediment          | 7,53 mg/kg |
| Onsite sewage treatment plant | 32 mg/l    |

### 8.2 Exposure controls

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### Skin protection

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)).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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)).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0,65 mm

Break through time: 10 min

Material tested: KCL 720 Camapren®

### **Body Protection**

Flame retardant antistatic protective clothing.

### **Respiratory protection**

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.

### **Control of environmental exposure**

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**

- |                                                 |                                                                   |
|-------------------------------------------------|-------------------------------------------------------------------|
| a) Physical state                               | clear, liquid                                                     |
| b) Color                                        | colorless                                                         |
| c) Odor                                         | ether-like                                                        |
| d) Melting point/freezing point                 | Melting point/range: -45,7 °C at 1.013 hPa                        |
| e) Initial boiling point and boiling range      | 81,0 - 82,0 °C at 1.013,25 hPa                                    |
| f) Flammability (solid, gas)                    | No data available                                                 |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 16 %(V)<br>Lower explosion limit: 4,4 %(V) |
| h) Flash point                                  | 2,0 °C - closed cup                                               |

- |                                           |                                                                                      |
|-------------------------------------------|--------------------------------------------------------------------------------------|
| i) Autoignition temperature               | 524,0 °C                                                                             |
| j) Decomposition temperature              | No data available                                                                    |
| k) pH                                     | No data available                                                                    |
| l) Viscosity                              | Viscosity, kinematic: No data available<br>Viscosity, dynamic: 0,350 Pas at 20,00 °C |
| m) Water solubility                       | 1.000 g/l at 25 °C completely soluble                                                |
| n) Partition coefficient: n-octanol/water | log Pow: -0,34                                                                       |
| o) Vapor pressure                         | 97,1 hPa at 20 °C                                                                    |
| p) Density                                | 0,786 g/cm <sup>3</sup> at 25 °C                                                     |
| Relative density                          | No data available                                                                    |
| q) Relative vapor density                 | No data available                                                                    |
| r) Particle characteristics               | No data available                                                                    |
|                                           |                                                                                      |
| s) Explosive properties                   | No data available                                                                    |
| t) Oxidizing properties                   | none                                                                                 |

## 9.2 Other safety information

- |                        |                      |
|------------------------|----------------------|
| Surface tension        | 29,0 mN/m at 20,0 °C |
| Relative vapor density | 1,42 - (Air = 1.0)   |

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 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 bases  
strong reducing agents  
Risk of explosion with:  
nitrates  
perchlorates  
perchloric acid  
conc. sulfuric acid  
with  
Heat.

Risk of ignition or formation of inflammable gases or vapours with:  
Oxidizing agents  
Nitric acid  
nitrogen dioxide  
with  
Catalyst  
Generates dangerous gases or fumes in contact with:  
Acids

#### **10.4 Conditions to avoid**

Extremes of temperature and direct sunlight.  
Warming.

#### **10.5 Incompatible materials**

rubber, various plastics, Strong oxidizing agents

#### **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 toxicity**

LD50 Oral - Mouse - male and female - 617 mg/kg

(OECD Test Guideline 401)

Acute toxicity estimate Oral - 617 mg/kg

(Calculation method)

LC50 Inhalation - Mouse - male and female - 4 h - 6,022 mg/l - vapor

(OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1.500 mg/kg

(Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

##### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

##### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Causes serious eye irritation.

(OECD Test Guideline 405)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

##### **Respiratory or skin sensitization**

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

##### **Germ cell mutagenicity**

Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation  
Result: negative  
Remarks: (ECHA)  
Test Type: In vitro mammalian cell gene mutation test  
Test system: Chinese hamster ovary cells  
Metabolic activation: with and without metabolic activation  
Method: US-EPA  
Result: negative  
Test Type: Mutagenicity (mammal cell test): chromosome aberration.  
Test system: Chinese hamster ovary cells  
Metabolic activation: with and without metabolic activation  
Result: Positive results were obtained in some in vitro tests.  
Remarks: (National Toxicology Program)  
Test Type: sister chromatid exchange assay  
Test system: Chinese hamster ovary cells  
Metabolic activation: Metabolic activation  
Result: negative  
Remarks: Sister chromatid exchange  
Test system: Saccharomyces cerevisiae  
Metabolic activation: without metabolic activation  
Result: positive  
Remarks: Cytogenetic analysis  
(ECHA)  
Test Type: In vitro mammalian cell gene mutation test  
Test system: Mouse lymphoma test  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 476  
Result: negative

Test Type: Micronucleus test  
Species: Mouse

Application Route: Intraperitoneal  
Method: OECD Test Guideline 474  
Result: negative

### **Carcinogenicity**

No evidence of carcinogenicity in animal studies.

### **Reproductive toxicity**

Animal testing did not show any effects on fertility.

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

The substance or mixture is not classified as specific target organ toxicant, single exposure.

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

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

### **Aspiration hazard**

No aspiration toxicity classification

## 11.2 Additional Information

### Endocrine disrupting properties

#### Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

RTECS: AL7700000

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish                      flow-through test LC50 - Pimephales promelas (fathead minnow) - 1.640 mg/l - 96 h  
Remarks: (ECHA)

Toxicity to algae                      static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253)  
static test ErC50 - Phaeodactylum tricornutum - 9.696 mg/l - 72 h (ISO 10253)

Toxicity to bacteria

Toxicity to fish(Chronic toxicity)                      flow-through test NOEC - Oryzias latipes - 102 mg/l - 21 d (OECD Test Guideline 204)

### 12.2 Persistence and degradability

Biodegradability                      Result: 70 % - Readily biodegradable. (OECD Test Guideline 310)

### 12.3 Bioaccumulative potential

No bioaccumulation is to be expected (log Pow <= 4).

### 12.4 Mobility in soil

Not expected to adsorb on soil.

### 12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### **12.6**

#### **Endocrine disrupting properties**

#### Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

## 12.7 Other adverse effects

Avoid release to the environment.

Stability in water DT50 - > 9.999 d pH 7 at 25 °C  
Remarks: (calculated)Hydrolyzes slowly.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 1648

IMDG: 1648

IATA: 1648

### 14.2 UN proper shipping name

ADR/RID: ACETONITRILE

IMDG: ACETONITRILE

IATA: Acetonitrile

### 14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

### 14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

### 14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

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## SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### Authorisations and/or restrictions on use

##### National legislation

Seveso III: Directive 2012/18/EU of the P5c FLAMMABLE LIQUIDS  
European Parliament and of the Council

on the control of major-accident hazards involving dangerous substances.

#### **Other regulations**

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

#### **15.2 Chemical Safety Assessment**

A Chemical Safety Assessment has been carried out for this substance.

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### **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.                                     |
| H302 + H312 + H332 | Harmful if swallowed, in contact with skin or if inhaled. |
| H312               | Highly flammable liquid and vapor.                        |
| H319               | Harmful if swallowed, in contact with skin or if inhaled. |
| H332               | Causes serious eye irritation.                            |

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## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

## Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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