# SAFETY DATA SHEET

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

Version 6.7
Revision Date 14.07.2026
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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 : Mettler-Toledo Calibration substance ME 18872, Caffeine

Product Number : 75035
Brand : Sigma-Aldrich
Index-No. : 613-086-00-5
REACH No. : 01-2119433305-48-XXXX
CAS-No. : 58-08-2

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

Identified uses : Laboratory chemicals, Manufacture of substances

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

Company : Merck Life Science S.A.S
80 Rue de Luzais
F-38297 SAINT QUENTIN FALLAVIER CEDEX

Telephone : +33 (0)1 85 16 94 34
E-mail address : servicetechnique@merckgroup.com

### 1.4 Emergency telephone number

Emergency Phone # : +33 (0)9 75 18 14 07 (CHEMTREC)
+33 (0)1 45 42 59 59 (I.N.R.S.)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

Acute toxicity, Category 4 H302: Harmful if swallowed.

### 2.2 Label elements

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



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Hazard pictograms :



Signal word : Warning

Hazard statements : H302 Harmful if swallowed.

Precautionary statements :

**Prevention:**

P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.

**Response:**

P301 + P312 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.

**Disposal:**

P501 Dispose of contents/ container to an approved waste disposal plant.

**Reduced Labelling (<= 125 ml)**

Hazard pictograms :



| | |
|---|---|
| Signal word | Warning |
| Hazard Statements | none |
| Precautionary Statements | 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.

Ecological information: 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.

Toxicological information: 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.

May form explosible dust-air mixture if dispersed.



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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Substance name : 1,3,7-Trimethylxanthine

Index-No. : 613-086-00-5

EC-No. : 200-362-1

**Components**

| Chemical name | CAS-No.<br>EC-No. | Concentration (% w/w) | M-Factor, SCL, ATE |
|---|---|---|---|
| Caffeine | 58-08-2<br>200-362-1 | >= 90 - <= 100 | Acute toxicity estimate<br><br>Acute oral toxicity: 367,7 mg/kg |

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air.

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

In case of eye contact : After eye contact: rinse out with plenty of water. 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 GHS label elements) 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 : Water



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| | | |
|---|---|---|
| media | | Foam<br>Carbon dioxide (CO2)<br>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

| | | |
|---|---|---|
| Specific hazards during fire fighting | : | Combustible.<br><br>Risk of dust explosion.<br>Development of hazardous combustion gases or vapours possible in the event of fire. |
| Hazardous combustion products | : | Carbon oxides<br><br>Nitrogen oxides (NOx) |

### 5.3 Advice for firefighters

| | | |
|---|---|---|
| Special protective equipment for fire-fighters | : | In the event of fire, wear self-contained breathing apparatus. |
| Further information | : | Suppress (knock down) gases/vapours/mists with a water spray jet.<br>Prevent fire extinguishing water from contaminating surface water or the ground water system. |

## SECTION 6: Accidental release measures

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

| | | |
|---|---|---|
| Personal precautions | : | Advice for non-emergency personnel:<br>Avoid inhalation of dusts.<br>Avoid substance contact.<br>Ensure adequate ventilation.<br>Evacuate the danger area, observe emergency procedures, consult an expert. |

Wear appropriate personal protective equipment, as indicated in Section 8.

### 6.2 Environmental precautions

| | | |
|---|---|---|
| Environmental precautions | : | Do not let product enter drains. |

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

| | | |
|---|---|---|
| Methods for cleaning up | : | Cover drains. Collect, bind, and pump off spills.<br>Observe possible material restrictions (see sections 7 and 10).<br>Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts. |

### 6.4 Reference to other sections



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For disposal considerations see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

| | | |
|---|---|---|
| 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 | : | Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance. |
| Temperature class | : | T1 |

For precautions see section 2 GHS label elements

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

| | | |
|---|---|---|
| Further information on storage conditions | : | Tightly closed. Dry. |
| Storage class (TRGS 510) | : | 11, Combustible Solids |
| Recommended storage temperature | : | 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

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

**Occupational Exposure Limits**

### 8.2 Exposure controls

**Individual protection measures, such as personal protective equipment (PPE)**

| | | |
|---|---|---|
| Eye/face protection | : | Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).<br>Safety glasses |

Hand protection

| | | |
|---|---|---|
| Material | : | Nitrile rubber |
| Break through time | : | 480 min |
| Glove thickness | : | 0,11 mm |
| Protective index | : | Full contact |
| Manufacturer | : | KCL 741 Dermatril® L |

| | | |
|---|---|---|
| Material | : | Nitrile rubber |
| Break through time | : | 480 min |
| Glove thickness | : | 0,11 mm |



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| | | |
|---|---|---|
| Protective index | : | Splash contact |
| Manufacturer | : | KCL 741 Dermatril® L |
| Remarks | : | 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de). |
| Skin and body protection | : | protective clothing |
| Respiratory protection | : | required when dusts are generated.<br><br>Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system. |
| Recommended Filter type: | : | Filter type P2 |

The entrepeneur 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**

| | | |
|---|---|---|
| Advice | : | Do not let product enter drains. |

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

| | | |
|---|---|---|
| Physical state | : | solid |
| Form | : | Crystalline powder |
| Colour | : | colourless |
| Odour | : | odourless |
| Odour Threshold | : | Not applicable |
| Melting point/ range | : | 234 - 236,5 °C |
| Boiling point | : | No data available |



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| | | |
|---|---|---|
| Flammability | : | May form combustible dust concentrations in air.<br><br>Remarks: The product is not flammable. |
| Upper explosion limit / Upper flammability limit | : | No data available |
| Lower explosion limit / Lower flammability limit | : | No data available |
| Flash point | : | Not applicable |
| Autoignition temperature | : | > 600 °C<br>Method: DIN 51794 |
| Decomposition temperature | : | No data available |
| pH | : | No data available |
| Viscosity, dynamic | : | No data available |
| Viscosity, kinematic | : | No data available |
| Flow time | : | No data available |
| Water solubility | : | No data available |
| Partition coefficient: n-octanol/water | : | No data available |
| Vapour pressure | : | No data available |
| Relative density | : | 1,23 (18 °C) |
| Density | : | 1,23 g/cm3 (18 °C) |
| Relative vapour density | : | No data available |

**9.2 Other information**

| | | |
|---|---|---|
| Explosives | : | Not classified as explosive. |
| Oxidizing properties | : | none |



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| | | |
|---|---|---|
| Burning rate | : | No data available |
| Evaporation rate | : | No data available |
| Molecular weight | : | 194,19 g/mol |

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

Hazardous reactions : Violent reactions possible with:

Strong oxidizing agents

### 10.4 Conditions to avoid

Conditions to avoid : no information available

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

**Acute toxicity**
LD50 Oral - Rat - male and female - 367,7 mg/kg
(OECD Test Guideline 401)
Remarks: (Regulation (EC) No 1272/2008, Annex VI)
Acute toxicity estimate Oral - 367,7 mg/kg
(ATE value derived from LD50/LC50 value)
LC50 Inhalation - Rat - male and female - 4 h - 4,94 mg/l - aerosol

(OECD Test Guideline 403)
LD50 Dermal - Rat - male and female - > 2.000 mg/kg
(OECD Test Guideline 402)

**Skin corrosion/irritation**
Skin - Rabbit
Result: No skin irritation - 4 h



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(OECD Test Guideline 404)

**Serious eye damage/eye irritation**
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

**Respiratory or skin sensitization**
Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)

**Germ cell mutagenicity**
Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Metabolic activation: without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: Human lymphocytes
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 473
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: Chinese hamster lung cells
Metabolic activation: without metabolic activation
Method: OECD Test Guideline 473
Result: positive

Test Type: Chromosome aberration test
Species: Mouse

Application Route: Intraperitoneal

Result: negative
Remarks: (ECHA)

Test Type: dominant lethal test
Species: Mouse

Application Route: Gavage

Result: negative
Remarks: (ECHA)

Test Type: Micronucleus test
Species: Mouse
Cell type: Red blood cells (erythrocytes)
Application Route: Oral
Method: OECD Test Guideline 474



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Result: Positive results were obtained in some in vivo tests.

Test Type: Chromosome aberration test
Species: Rat

Application Route: Oral

Result: negative
Remarks: (ECHA)

**Carcinogenicity**
No data available

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
No data available

## 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. |

Repeated dose toxicity - Mouse - male and female - Oral - 90 d - No observed adverse effect level - 167,4 - 179,4 mg/kg
Remarks: (ECHA)

RTECS: EV6475000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption of toxic quantities:

Diarrhoea
Vomiting
agitation
Headache

Systemic effects:

drop in blood pressure
tachycardia
collapse



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Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

## SECTION 12: Ecological information

### 12.1 Toxicity

**Components:**

**Caffeine:**

| | | |
|---|---|---|
| Toxicity to fish | : | LC50 (Leuciscus idus (Golden orfe)): ca. 87 mg/l<br>End point: mortality<br>Exposure time: 96 h<br>Test Type: static test<br>Method: DIN 38412 part 15<br><br>NOEC (Leuciscus idus (Golden orfe)): 46 mg/l<br>End point: mortality<br>Exposure time: 96 h<br>Test Type: static test<br>Method: DIN 38412 part 15 |
| Toxicity to daphnia and other aquatic invertebrates | : | EC50 (Daphnia magna (Water flea)): 182 mg/l<br>End point: mortality<br>Exposure time: 48 h<br>Test Type: static test<br>Method: DIN 38412 |
| Toxicity to algae/aquatic plants | : | ErC50 (Desmodesmus subspicatus (green algae)): > 100 mg/l<br>Exposure time: 72 h<br>Test Type: static test<br>Analytical monitoring: yes<br>Method: OECD Test Guideline 201<br>GLP: yes |
| Toxicity to microorganisms | : | EC50 (activated sludge): > 1.000 mg/l<br>Exposure time: 3 h<br>Method: OECD Test Guideline 209<br>GLP: yes |

**Ecotoxicology Assessment**

| | | |
|---|---|---|
| Chronic aquatic toxicity | : | This product has no known ecotoxicological effects. |

### 12.2 Persistence and degradability

**Components:**

**Caffeine:**

| | | |
|---|---|---|
| Biodegradability | : | Test Type: aerobic |



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Inoculum: activated sludge
Concentration: 43 mg/l
Result: Readily biodegradable.
Biodegradation: 90 - 100 %
Exposure time: 22 d
Method: OECD Test Guideline 301A
GLP: yes

### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

**Product:**

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

**Components:**

**Caffeine:**

Additional ecological information : Discharge into the environment must be avoided.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

Product : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

## SECTION 14: Transport information

### 14.1 UN number or ID number



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| | | |
|---|---|---|
| **ADR** | : | Not regulated as a dangerous good |
| **IMDG** | : | Not regulated as a dangerous good |
| **IATA_P** | : | Not regulated as a dangerous good |

**14.2 UN proper shipping name**

| | | |
|---|---|---|
| **ADR** | : | Not regulated as a dangerous good |
| **IMDG** | : | Not regulated as a dangerous good |
| **IATA_P** | : | Not regulated as a dangerous good |

**14.3 Transport hazard class(es)**

| | | |
|---|---|---|
| **ADR** | : | Not regulated as a dangerous good |
| **IMDG** | : | Not regulated as a dangerous good |
| **IATA_P** | : | Not regulated as a dangerous good |

**14.4 Packing group**

| | | |
|---|---|---|
| **ADR** | : | Not regulated as a dangerous good |
| **IMDG** | : | Not regulated as a dangerous good |
| **IATA (Cargo)** | : | Not regulated as a dangerous good |
| **IATA_P (Passenger)** | : | Not regulated as a dangerous good |

**14.5 Environmental hazards**

Not regulated as a dangerous good

**14.6 Special precautions for user**

| | | |
|---|---|---|
| Remarks | : | Not classified as dangerous in the meaning of transport regulations. |

**14.7 Maritime transport in bulk according to IMO instruments**

Not applicable for product as supplied.

## SECTION 15: Regulatory information

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

| | | |
|---|---|---|
| REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII) | : | Conditions of restriction for the following entries should be considered:<br>Number on list 3: Caffeine |
| REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59). | : | Not applicable |
| Regulation (EU) No 2024/590 on substances that deplete the ozone layer | : | Not applicable |
| Regulation (EU) 2019/1021 on persistent organic | : | Not applicable |



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pollutants (recast)

| | | |
|---|---|---|
| REACH - List of substances subject to authorisation (Annex XIV) | : | Not applicable |
| Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances. | | Not applicable |

### 15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

## SECTION 16: Other information

### Full text of H-Statements

### Full text of other abbreviations

Acute Tox. : Acute toxicity

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; CLP - Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECHA - European Chemicals Agency; EC-Number - European Community number; 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 Harmonised 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 Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; 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 - Organisation 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; SVHC - Substance of Very High



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Concern; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TRGS - Technical Rule for Hazardous Substances; TSCA - Toxic Substances Control Act (United States); UN - United Nations; vPvB - Very Persistent and Very Bioaccumulative

**Further information**

Other information : The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
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