

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.3

Revision Date 24.02.2021

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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 : Caffeine

Product Number : W222402

Brand : 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.r.l.
Via Monte Rosa 93
I-20149 MILANO

Telephone : +39 02 3341 7340

Fax : +39 02 3801 0737

E-mail address : serviziotecnico@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : 800-789-767 (CHEMTREC Italia)
+39-02-4555-7031 (CHEMTREC chiamate internazionali)
+39 02-6610-1029 (Centro Antiveleni Niguarda Ca' Granda - Milano)

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****Classification according to Regulation (EC) No 1272/2008**

Acute toxicity, Oral (Category 4), H302

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

Warning



| | |
|--|---|
| Hazard statement(s) H302 | Harmful if swallowed. |
| Precautionary statement(s) P301 + P312 + P330 | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth. |
| Supplemental Hazard Statements | none |
| Reduced Labeling (<= 125 ml) | |
| Pictogram |  |
| Signal word | Warning |
| 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.

SECTION 3: Composition/information on ingredients

3.1 Substances

| | | |
|------------------|---|--|
| Synonyms | : | 1,3,7-Trimethylxanthine |
| Formula | : | C ₈ H ₁₀ N ₄ O ₂ |
| Molecular weight | : | 194,19 g/mol |
| CAS-No. | : | 58-08-2 |
| EC-No. | : | 200-362-1 |
| Index-No. | : | 613-086-00-5 |

| Component | Classification | Concentration |
|------------------------|--------------------|---------------|
| Caffeine | | |
| CAS-No. 58-08-2 | Acute Tox. 4; H302 | <= 100 % |
| EC-No. 200-362-1 | | |
| Index-No. 613-086-00-5 | | |

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

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



If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.



SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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. Store in cool place.

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

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)



data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: Crystalline powder Color: colorless |
| b) Odor | odorless |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 234 - 236,5 °C - lit. |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | No data available |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | The product is not flammable. |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapor pressure | No data available |
| l) Vapor density | No data available |
| m) Relative density | 1,23 at 18 °C |
| n) Water solubility | 18,7 g/l at 16 °C |
| o) Partition coefficient: | log Pow: -0,091 at 23 °C - Bioaccumulation is not expected. |



- n-octanol/water
- p) Autoignition temperature No data available
- q) Decomposition temperature No data available
- r) Viscosity Viscosity, kinematic: No data available
Viscosity, dynamic: No data available
- s) Explosive properties No data available
- t) Oxidizing properties No data available

9.2 Other safety information

Dissociation constant 10,4 at 40 °C

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

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)

LC50 Inhalation - Rat - male and female - 4 h - 4,94 mg/l
(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



(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

In vitro mammalian cell gene mutation test

mouse lymphoma cells

Result: negative

Chromosome aberration test in vitro

Human lymphocytes

Result: negative

Ames test

Escherichia coli/Salmonella typhimurium

Result: negative

Chromosome aberration test in vitro

Chinese hamster lung cells

Result: positive

Mouse - male

Result: negative

Remarks:

(ECHA)

Human

Result: negative

Remarks:

(ECHA)

Mouse - male

Result: negative

Remarks:

(ECHA)

OECD Test Guideline 474

Mouse - male and female - Red blood cells (erythrocytes)

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

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

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

Repeated dose toxicity - Mouse - male and female - Oral - 90 d - NOAEL (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:

Diarrhea
Vomiting
agitation
Headache

Systemic effects:

drop in blood pressure
tachycardia

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

| | |
|---|--|
| Toxicity to fish | static test LC50 - Leuciscus idus (Golden orfe) - ca. 87 mg/l - 96 h (DIN 38412 part 15) |
| | static test NOEC - Leuciscus idus (Golden orfe) - 46 mg/l - 96 h (DIN 38412 part 15) |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - 182 mg/l - 48 h (DIN 38412) |
| Toxicity to algae | static test ErC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201) |
| | static test NOEC - Desmodesmus subspicatus (green algae) - 6,25 mg/l - 72 h (OECD Test Guideline 201) |
| Toxicity to bacteria | EC50 - activated sludge - > 1.000 mg/l - 3 h (OECD Test Guideline 209) |



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.

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, preparations and articles (Annex XVII) : Not applicable

National legislation

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 referred to under sections 2 and 3.

H302 Harmful if swallowed.

Further information

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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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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