

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 5.5 Revision Date 13.06.2014

Print Date 14.05.2018

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	:	C0750
Brand	:	Sigma-Aldrich
Index-No.	:	613-086-00-5
REACH No.	:	A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
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 :

1.4 Emergency telephone number

Emergency Phone # :

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.

Classification according to EU Directives 67/548/EEC or 1999/45/EC

Xn Harmful R22

For the full text of the R-phrases 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)	none
Supplemental Hazard Statements	none

2.3 Other hazards - none

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

Hazardous ingredients according to Regulation (EC) No 1272/2008

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

Hazardous ingredients according to Directive 1999/45/EC

Component	Classification	Concentration
Caffeine		
CAS-No. 58-08-2 EC-No. 200-362-1 Index-No. 613-086-00-5	Xn, R22	<= 100 %

For the full text of the H-Statements and R-Phrases 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 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**
no data available
- 5.3 Advice for firefighters**
Wear self contained breathing apparatus for fire fighting 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 vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.
For personal protection see section 8.
- 6.2 Environmental precautions**
Do not let product enter drains.
- 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**
Avoid contact with skin and eyes. Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed.
For precautions see section 2.2.
- 7.2 Conditions for safe storage, including any incompatibilities**
Store in cool place. Keep container tightly closed in a dry and well-ventilated 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**
Components with workplace control parameters
- 8.2 Exposure controls**
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
- 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 EU Directive 89/686/EEC 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: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0,11 mm
Break through time: 480 min
Material tested: Dermatrill® (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 CE 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

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|--|
| a) Appearance | Form: powder
Colour: white |
| b) Odour | odourless |
| c) Odour Threshold | no data available |
| d) pH | 5,5 - 6,5 at 10 g/l at 20 °C |
| 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) | no data available |
| j) Upper/lower flammability or explosive limits | no data available |
| k) Vapour pressure | 20 hPa at 89 °C |
| l) Vapour density | no data available |
| m) Relative density | 1,230 g/cm ³ at 18 °C |
| n) Water solubility | 18,7 g/l at 16 °C |
| o) Partition coefficient: n-octanol/water | log Pow: -0,091 at 23 °C |

- | | | |
|----|---------------------------|-------------------|
| p) | Auto-ignition temperature | no data available |
| q) | Decomposition temperature | no data available |
| r) | Viscosity | no data available |
| s) | Explosive properties | no data available |
| t) | Oxidizing properties | no data available |

9.2 Other safety information

Bulk density	220 kg/m ³
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

Other decomposition products - no data available
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)

LC50 Inhalation - rat - male and female - 4,94 mg/l
(Calculation method)

LD50 Dermal - rat - male and female - > 2.000 mg/kg

Skin corrosion/irritation

Skin - rabbit

Result: No skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - rabbit

Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitisation

- mouse

Result: Did not cause sensitisation on laboratory animals.

Germ cell mutagenicity

rat
Kidney
Micronucleus test

mouse
Micronucleus test

Carcinogenicity

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Caffeine)

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

Additional Information

RTECS: EV6475000

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

Liver - Irregularities - Based on Human Evidence

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	LC50 - Leuciscus idus (Golden orfe) - 87 mg/l - 96 h
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 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

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

12.6 Other adverse effects

no data available

SECTION 13: Disposal considerations**13.1 Waste treatment methods****Product**

Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

SECTION 14: Transport information

14.1 UN number			
ADR/RID: -	IMDG: -		IATA: -
14.2 UN proper shipping name			
ADR/RID: Not dangerous goods			
IMDG: Not dangerous goods			
IATA: Not dangerous goods			
14.3 Transport hazard class(es)			
ADR/RID: -	IMDG: -		IATA: -
14.4 Packaging group			
ADR/RID: -	IMDG: -		IATA: -
14.5 Environmental hazards			
ADR/RID: no	IMDG Marine pollutant: no		IATA: no
14.6 Special precautions for user			
no data available			

SECTION 15: Regulatory information

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

- 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
- no data available
- 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.

Acute Tox.	Acute toxicity
H302	Harmful if swallowed.

Full text of R-phrases referred to under sections 2 and 3

Xn	Harmful
R22	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.