



# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.4

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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 : 56396

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

### 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

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)<br>H302        | Harmful if swallowed.                                               |
| Precautionary statement(s)<br>P264 | Wash skin thoroughly after handling.                                |
| P270                               | Do not eat, drink or smoke when using this product.                 |
| P301 + P312                        | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.      |
| P501                               | Dispose of contents/ container to an approved waste disposal plant. |
| 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

|                  |                                                                |
|------------------|----------------------------------------------------------------|
| Formula          | : C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> |
| 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 |
|------------------------|--------------------|---------------|
| <b>Caffeine</b>        |                    |               |
| 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.

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## 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.

#### 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 2.2) and/or in section 11

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

No data available

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## 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.

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

### 5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

### 5.4 Further information

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: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. 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.

### 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### 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

For precautions see section 2.2.

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

#### Storage conditions

Tightly closed. Dry.

#### Storage stability

Recommended storage temperature  
15 - 25 °C

Store under inert gas. Moisture sensitive.

#### Storage class

Storage class (TRGS 510): 11: Combustible Solids

### 7.3 Specific end use(s)

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

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## 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

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: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

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: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

### **Body Protection**

protective clothing

### **Respiratory protection**

required when dusts are generated.

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 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.

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## **SECTION 9: Physical and chemical properties**

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

- |                                            |                   |
|--------------------------------------------|-------------------|
| a) Physical state                          | powder            |
| b) Color                                   | white, colorless  |
| c) Odor                                    | odorless          |
| d) Melting point/freezing point            | No data available |
| e) Initial boiling point and boiling range | No data available |

|                                                 |                                                                                  |
|-------------------------------------------------|----------------------------------------------------------------------------------|
| f) Flammability (solid, gas)                    | No data available                                                                |
| g) Upper/lower flammability or explosive limits | No data available                                                                |
| h) Flash point                                  | No data available                                                                |
| i) Autoignition temperature                     | No data available                                                                |
| j) Decomposition temperature                    | No data available                                                                |
| k) pH                                           | No data available                                                                |
| l) Viscosity                                    | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                             | No data available                                                                |
| n) Partition coefficient: n-octanol/water       | No data available                                                                |
| o) Vapor pressure                               | No data available                                                                |
| p) Density                                      | 1,23 g/cm <sup>3</sup> at 18 °C                                                  |
| Relative density                                | 1,23 at 18 °C                                                                    |
| q) Relative vapor density                       |                                                                                  |
| r) Particle characteristics                     | No data available                                                                |
| s) Explosive properties                         | No data available                                                                |
| t) Oxidizing properties                         | none                                                                             |

## 9.2 Other safety information

No data available

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## 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

Violent reactions possible with:  
Strong oxidizing agents

#### 10.4 Conditions to avoid

no information available

#### 10.5 Incompatible materials

no information available

#### 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 - 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 - 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

(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: 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: 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: Chinese hamster lung cells  
Metabolic activation: without metabolic activation  
Method: OECD Test Guideline 473  
Result: positive

Test Type: Mutagenicity (mammal cell test): chromosome aberration.  
Species: Mouse

Application Route: Intraperitoneal

Result: negative  
Remarks: (ECHA)

Test Type: Mutagenicity (mammal cell test): chromosome aberration.  
Species: Human

Application Route: Oral

Result: negative  
Remarks: (ECHA)

Test Type: dominant lethal test  
Species: Mouse

Application Route: Oral

Result: negative  
Remarks: (ECHA)

Test Type: Micronucleus test  
Species: Mouse  
Cell type: Red blood cells (erythrocytes)  
Application Route: Oral  
Method: OECD Test Guideline 474  
Result: Positive results were obtained in some in vivo tests.

**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 - 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

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## 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)

#### 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 22 d  
Result: 90 - 100 % - Readily biodegradable.  
(OECD Test Guideline 301A)

#### 12.3 Bioaccumulative potential

No data available

#### 12.4 Mobility in soil

No data available

#### 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

Discharge into the environment must be avoided.

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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: -

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

##### Further information

Not classified as dangerous in the meaning of transport regulations.

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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.

##### 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

For this product a chemical safety assessment was not carried out

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### SECTION 16: Other information

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

H302 Harmful if swallowed.

## 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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