

## SAFETY DATA SHEET

Version 6.5  
Revision Date 01/15/2020  
Print Date 11/20/2020**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

CAS-No. : 58-08-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

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

Company : Sigma-Aldrich Inc.  
3050 Spruce Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

**1.4 Emergency telephone number**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 4), H302  
Short-term (acute) aquatic hazard (Category 3), H402

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

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word : Warning

Hazard statement(s)  
H302 : Harmful if swallowed.

H402	Harmful to aquatic life.
Precautionary statement(s)	
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P501	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

---

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	: 1,3,7-Trimethylxanthine
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>		
	Acute Tox. 4; Aquatic Acute 3; H302, H402	<= 100 %

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 safety data sheet to the doctor in attendance. Move out of dangerous area.

#### 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<sub>x</sub>)

#### **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 vapours, 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**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

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**

Keep container tightly closed in a dry and well-ventilated place.

Keep in a dry place.

Storage class (TRGS 510): 13: Non Combustible Solids

### 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

Contains no substances with occupational exposure limit values.

### 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.

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 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

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: powder<br>Colour: colourless                                  |
| b) Odour  | odourless   |
| c) Odour Threshold                              | No data available   |
| d) pH   | No data available   |
| e) Melting point/freezing point                 | Melting point/range: 234 - 236.5 °C (453 - 457.7 °F) - 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) Vapour pressure                              | No data available   |
| l) Vapour density                               | No data available   |
| m) Relative density                             | 1.23 g/cm <sup>3</sup> at 18 °C (64 °F)                             |
| n) Water solubility                             | 18.7 g/l at 16 °C (61 °F)   |
| o) Partition coefficient: n-octanol/water       | log Pow: -0.091 at 23 °C (73 °F) - Bioaccumulation is not expected. |
| 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

Dissociation constant 10.4 at 40 °C (104 °F)

---

## 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

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

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)

No data available

#### 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 sensitisation

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  
(ECHA)

Human  
Result: negative  
(ECHA)

Mouse - male  
Result: negative  
(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 component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **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**

Repeated dose toxicity - Mouse - male and female - Oral - 90 d - No observed adverse effect level - 167.4 - 179.4 mg/kg  
(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

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

---

## SECTION 12: Ecological information

### 12.1 Toxicity

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

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

### 12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life.

Discharge into the environment must be avoided.

---

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

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

**Contaminated packaging**

Dispose of as unused product.

---

**SECTION 14: Transport information****DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

---

**SECTION 15: Regulatory information****SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

Caffeine	CAS-No. 58-08-2	Revision Date
----------	--------------------	---------------

Caffeine	CAS-No. 58-08-2	Revision Date
----------	--------------------	---------------

---

**SECTION 16: Other information**

**Further information**

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.5

Revision Date: 01/15/2020

Print Date: 11/20/2020