

# SAFETY DATA SHEET

Version 6.8  
Revision Date 03/31/2026  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : Caffeine

Product Number : 56396  
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

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
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

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## SECTION 2. HAZARDS IDENTIFICATION

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

#### Hazards for the product as supplied

Acute toxicity (Oral) : Category 4

Short-term (acute) aquatic hazard : Category 3

### Other hazards

None known.

### GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : H302 Harmful if swallowed.  
H402 Harmful to aquatic life.

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

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## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 58-08-2

### Components

| Chemical name | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|---------------|-------------------|-----------------------|--------------|
| Caffeine      | 58-08-2*          | >= 90 - <= 100        | -            |

\* Indicates that the identifier is a CAS No.  
Actual concentration is withheld as a trade secret

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## SECTION 4. FIRST AID MEASURES

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

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|   |   |
|---|---|
|   | 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.                   |
| 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 |
| Protection of first-aiders                                  | : For personal protection see section 8.  |
| Notes to physician  | : No data available   |

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## SECTION 5. FIREFIGHTING MEASURES

|                                       |   |
|---------------------------------------|---|
| Suitable extinguishing media          | : Water<br>Foam<br>Carbon dioxide (CO <sub>2</sub> )<br>Dry powder  |
| Unsuitable extinguishing media        | : For this substance/mixture no limitations of extinguishing agents are given.                            |
| Specific hazards during fire fighting | : Combustible.<br><br>Development of hazardous combustion gases or vapours possible in the event of fire. |
| Hazardous combustion products         | : Carbon oxides<br><br>Nitrogen oxides (NO <sub>x</sub> )   |
| Specific extinguishing methods        | : No data available   |
| Further information                   | : Suppress (knock down) gases/vapours/mists with a water spray jet.                                       |

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : In the event of fire, wear self-contained breathing apparatus.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

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.  
Advice for emergency responders:  
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.

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.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions : Tightly closed.  
Dry.

Storage class : 11, Combustible Solids

Recommended storage temperature : 59 - 77 °F / 15 - 25 °C

Further information on storage stability : Store under inert gas.  
Moisture sensitive.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### **Personal protective equipment**

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.

#### 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  
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](http://www.kcl.de)).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : powder

Color : white, colourless

Odor : odourless

Odor Threshold : Not applicable

pH : No data available

Melting point : No data available

Boiling point/boiling range : No data available

Flash point : No data available

Evaporation rate : No data available

Burning rate : No data available

Upper explosion limit /  
Upper flammability limit : No data available

Lower explosion limit /  
Lower flammability limit : No data available

Vapor pressure : No data available

Relative vapour density : No data available

Relative density : 1.23 (64 °F / 18 °C)

Density : 1.23 g/cm<sup>3</sup> (64 °F / 18 °C)

Water solubility : No data available

Partition coefficient: n-  
octanol/water : No data available

Autoignition temperature : > 1112 °F / > 600 °C  
Method: DIN 51794

|                           |                     |
|---------------------------|---------------------|
| Decomposition temperature | : No data available |
| Viscosity, dynamic        | : No data available |
| Viscosity, kinematic      | : No data available |
| Flow time                 | : No data available |
| Explosive properties      | : No data available |
| Oxidizing properties      | : none              |
| Molecular weight          | : 194.19 g/mol      |
| Particle characteristics  |                     |
| Particle size             | : No data available |

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## SECTION 10. STABILITY AND REACTIVITY

|                                    |   |
|------------------------------------|---|
| 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. |
| Chemical stability                 | : The product is chemically stable under standard ambient conditions (room temperature) .   |
| Possibility of hazardous reactions | : Violent reactions possible with:<br>Strong oxidizing agents   |
| Conditions to avoid                | : no information available  |
| Incompatible materials             | : no information available  |
| 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: 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  
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**

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

## **11.2 Additional Information**

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

Handle in accordance with good industrial hygiene and safety practice.

Liver - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

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## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

##### **Caffeine:**

- Toxicity to fish : LC50 (Leuciscus idus (Golden orfe)): ca. 87 mg/l  
End point: mortality  
Exposure time: 96 h  
Test Type: static test  
Method: DIN 38412 part 15
- NOEC (Leuciscus idus (Golden orfe)): 46 mg/l  
End point: mortality  
Exposure time: 96 h  
Test Type: static test  
Method: DIN 38412 part 15
- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 182 mg/l  
End point: mortality  
Exposure time: 48 h  
Test Type: static test  
Method: DIN 38412
- Toxicity to algae/aquatic plants : ErC50 (Desmodesmus subspicatus (green algae)): > 100 mg/l  
Exposure time: 72 h  
Test Type: static test  
Analytical monitoring: yes  
Method: OECD Test Guideline 201  
GLP: yes
- Toxicity to microorganisms : EC50 (activated sludge): > 1,000 mg/l  
Exposure time: 3 h  
Method: OECD Test Guideline 209

GLP: yes

### **Ecotoxicology Assessment**

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

### **Persistence and degradability**

#### **Components:**

##### **Caffeine:**

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

### **Bioaccumulative potential**

No data available

### **Mobility in soil**

No data available

### **Other adverse effects**

#### **Components:**

##### **Caffeine:**

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

### **Endocrine disrupting properties**

No data available

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## **SECTION 13. DISPOSAL CONSIDERATIONS**

### **Disposal methods**

Waste from residues : 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.

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## **SECTION 14. TRANSPORT INFORMATION**

### **International Regulations**

#### **IATA-DGR**

Not regulated as a dangerous good

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**IMDG-Code**

Not regulated as a dangerous good

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

**National Regulations****49 CFR**

Not regulated as a dangerous good

Poison Inhalation Hazard : No

**Special precautions for user**

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

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**SECTION 15. REGULATORY INFORMATION****CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard  
Chronic Health Hazard

**SARA 313** : 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.

**US State Regulations****Massachusetts Right To Know**

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

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The components of this product are reported in the following inventories:**

US TSCA : All substances listed as active on the TSCA inventory

## **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; 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; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; 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; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; 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; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; 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

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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for

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