

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.12
Revision Date 06/05/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : CAFFEINE

Product Number : 27602
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

SECTION 2. HAZARDS IDENTIFICATION

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

Hazards for the product as supplied

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Combustible dust

Acute toxicity (Oral) : Category 4

Short-term (acute) aquatic hazard : Category 3

Other hazards

May form explosible dust-air mixture if dispersed.

GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : May form combustible dust concentrations in air.
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.

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*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range 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 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

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.

Risk of dust explosion.

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

Hazardous combustion products	: Carbon oxides Nitrogen oxides (NO _x)
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.

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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	: Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Further information on storage conditions	: Tightly closed. Dry.

Storage class : 11, Combustible Solids

Recommended storage temperature : Recommended storage temperature see product label.

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).

- 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.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : Crystalline powder
- Color : colourless
- Odor : odourless
- Odor Threshold : Not applicable
- pH : No data available
- Melting point/ range : 453 - 457.7 °F / 234 - 236.5 °C
- Boiling point/boiling range : No data available
- Flash point : Not applicable
- Evaporation rate : No data available
- Flammability (solid, gas) : May form combustible dust concentrations in air.
- 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

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Relative vapour density	: No data available
Relative density	: 1.23 (64 °F / 18 °C)
Density	: 1.23 g/cm ³ (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	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 194.19 g/mol
Particle characteristics	
Particle size	: No data available

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: Strong oxidizing agents
Conditions to avoid	: no information available
Incompatible materials	: No data available

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

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 : EC50 (Daphnia magna (Water flea)): 182 mg/l
End point: mortality

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invertebrates	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

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

Caffeine:

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

Endocrine disrupting properties

No data available

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.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

Not regulated as a dangerous good

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.

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 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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. Clean Water Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean Water Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

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.

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

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

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