

Chemical Safety Data Sheet MSDS / SDS

Caffeine SDS

Revision Date:2024-04-25 Revision Number:1

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name: Caffeine
CAS: 58-08-2

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.
Uses advised against: none

Company Identification

Company: Chemicalbook.in
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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 4, Oral

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H302 Harmful if swallowed

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

Storage

none

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name: Caffeine

Common names and synonyms: Caffeine

CAS number: 58-08-2
EC number: 200-362-1
Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Refer for medical attention .

Most important symptoms/effects, acute and delayed

SYMPTOMS: Symptoms of exposure to this compound may include central nervous system stimulation, less drowsiness, less fatigue, more rapid and clearer flow of thought, decreased reaction time, affects on muscular coordination, accurate timing and arithmetic skills, nervousness, restlessness, insomnia, tremors and hyperesthesia. At higher doses, symptoms include focal and generalized convulsions, Cheyne-Stokes respiration, apnea of preterm infants, vomiting, nausea, effects on circulatory system, small decreases in heart rate, tachycardia, arrhythmias, premature ventricular contractions and vasodilation. Overdosage may cause death, emesis, convulsions, excitement, mild delirium, sensory disturbances such as ringing in the ears and flashes of light, tense and tremulous muscles, extrasystoles and quickened respiration. Continued excessive use may lead to digestive disturbances, constipation, palpitations, shortness of breath and depressed mental states. Other symptoms may include pulmonary edema, myocardial infarction, ventricular fibrillation, stomach cramps, chills, cerebral edema and hypokalemia. It may also cause rapid pulse, hallucinations, photophobia, gastroenteric distress and diuresis. Anxiety and irritability may occur. Gastric irritation, headache, fever, agitation, hyperventilation and respiratory failure may also occur. Dizziness has been reported. It may also cause irritation of the skin, eyes, mucous membranes and respiratory tract. **ACUTE/CHRONIC HAZARDS:** This compound is harmful by ingestion, inhalation or skin absorption. It is an irritant of the skin, eyes, mucous membranes and respiratory tract. When heated to decomposition it emits toxic fumes of carbon monoxide, carbon dioxide and nitrogen oxides. (NTP, 1992)

Indication of immediate medical attention and special treatment needed, if necessary

Emergency and supportive measures: Maintain an open airway and assist ventilation if necessary. Treat seizures and hypotension if they occur. Extreme anxiety or agitation may respond to benzodiazepines such as IV lorazepam. Hypokalemia usually resolves without treatment but in severe poisonings may need treatment as it can contribute to life-threatening arrhythmias. Monitor ECG and vital signs for at least 6 hours after ingestion.

SECTION 5: Firefighting measures

Suitable extinguishing media

Use water spray, powder.

Specific hazards arising from the chemical

Flash point data for this chemical are not available; however, it is probably combustible. (NTP, 1992)

Special protective actions for fire-fighters

Use water spray, dry powder.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs. Well closed. Separated from food and feedstuffs. Well closed.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Caffeine			
CAS No.	58-08-2			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m ³	ppm	mg/m ³
Latvia	?	0,5	?	?
	Remarks			

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	PHYSICAL DESCRIPTION: Odorless white powder or white glistening needles, usually melted together. Bitter taste. Solutions in water are neutral to litmus. Odorless. (NTP, 1992)
Colour:	White, prismatic crystals
Odour:	Odorless
Melting point/freezing point:	234-236.5°C(lit.)
Boiling point or initial boiling point and boiling range:	178°C
Flammability:	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	178°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	pH = 6.9 (1% solution)
Kinematic viscosity:	no data available

Solubility:	10 to 50 mg/mL at 73° F (NTP, 1992)
Partition coefficient n-octanol/water:	-0.07
Vapour pressure:	9.0X10-7 mm Hg at 25 deg C /Extrapolated/
Density and/or relative density:	1.23
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic fumes including nitrogen oxides.

Chemical stability

no data available

Possibility of hazardous reactions

Combustible. CAFFEINE may be hygroscopic. Aqueous solutions (1.12 mg/mL) are stable for three weeks at 41° F if protected from light. In normal room lighting and at room temperature, solutions are stable for 3 days. Solutions of this chemical in water, DMSO, 95% ethanol or acetone should be stable for 24 hours under normal lab conditions. REACTIVITY: This compound may react with strong oxidizing agents. It is also incompatible with iodine, silver salts and tannins. This compound is a very weak base. It is decomposed by strong solutions of caustic alkalis. (NTP, 1992)

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition, it emits toxic fumes of /nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat oral 192 mg/kg

Inhalation: no data available

Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Evaluation: There is inadequate evidence for the carcinogenicity in humans of caffeine. There is inadequate evidence for the carcinogenicity in experimental animals of caffeine. Overall evaluation: Caffeine is not classifiable as to its carcinogenicity to humans (Group 3).

Reproductive toxicity

no data available

STOT-single exposure

The substance may cause effects on the central nervous system and cardiovascular system. This may result in insomnia, excitement, tachycardia and polyuria.

STOT-repeated exposure

no data available

Aspiration hazard

Evaporation at 20°C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: *Pimephales promelas* (Fathead minnow); Conditions: freshwater, static; Concentration: 100 mg/L for 48 hr

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: *Daphnia magna* (Water flea) age < 24 hr neonate; Conditions: freshwater, static, 21 deg C; Concentration: 3.521 mM for 24 hr; Effect: intoxication, immobilization

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: The estimated half-life for caffeine in the Rhine River, Netherlands, was 0.8 days, which was thought to occur as a result of biological removal processes(1). Caffeine was found to be readily biodegradable when incubated with a sewage sludge inoculum(2). Using OECD 301F method, biodegradation was found to be 58% in one vessel and 84% in a second vessel(3). The structurally analogous substance theophylline (differs by only one methyl group from caffeine) is readily biodegradable by OECD 301A method with 90-100% biodegradation after 22 days and >90% at the end of the 10-days-window(3). In biodegradation studies using 3 soils from Ontario Canada and a 34-day incubation period, ¹⁴C-caffeine was rapidly mineralized to ¹⁴C-CO₂ in a sandy loam and loam soil, and less rapidly in a silt loam soil(4); mineralization in the sandy loam and loam soils reached about 60% in 20 days (50% in 3-10 days) with mineralization in the silt loam soil reaching about 25% in 34 days(4). A microcosm study using sediments collected upstream and downstream from wastewater treatment plants found caffeine to undergo biomineralization under aerobic conditions(5).

Bioaccumulative potential

An estimated BCF of 3 was calculated for caffeine in fish(SRC), using a log Kow of -0.07(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The log Koc of caffeine was experimentally determined to be 2.87 and 3.89 in a silt loam soil and in a sandy loam soil respectively(1). According to a classification scheme(2), a log Koc range of 2.87 to 3.89 (Koc range of 741 to 7762) suggests that caffeine may have low mobility in soil to being immobile in soil. Sorption tests using sand approximated a log Koc value of 1.85 (Koc of 71) using an assumed organic carbon content of 0.1% in the sand(1) which would suggest high mobility(2,SRC). Caffeine is both a weak acid and a weak base with pKa values of 14.0(3) and 0.7(4). Although partial ionization to cation and anion forms may occur, electrochemical studies have found that the neutral form of caffeine was predominant in the pH range of 5.5 to 9.0(4). Cations generally adsorb more strongly to organic carbon and clay than their neutral counterparts(5) suggesting that the cation form of caffeine may have higher Koc values than the neutral form(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1544 (For reference only, please check.)

IMDG: UN1544 (For reference only, please check.)

IATA: UN1544 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

IMDG: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

IATA: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer: 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. We as supplier shall not be held liable for any