

SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: Caffeine
CAS number: 58-08-2
Synonyms: 1,3,7-trimethylxanthine, 1,3,7-Trimethylpurine-2,6-dione

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 : Lab Alley, LLC
22111 Highway 71 West, Suite 601
Spicewood, Texas 78669
U.S.A.

Telephone : 512-668-9918
Fax : 512-886-4008

1.4 Emergency telephone

Emergency Phone # : US & Canada: 1-800-535-5053 INFOTRAC
International 1-352-323-3500 INFOTRAC

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)
Short-term (acute) aquatic hazard (Category 3)

2.2 GHS Label elements, including precautionary statements

Pictogram:



Signal Word:

Warning

Hazard statement(s):

Harmful if swallowed. Harmful to aquatic life.

Precautionary statement(s):

Prevention - Wash skin thoroughly after handling. Do not eat, drink or smoke when using this product. Avoid release into the environment. **Response** - IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Dispose of contents/container to an approved waste disposal plant.

Hazards not otherwise classified

None.

SECTION 3: Composition/information on ingredients

3.1 Components

Ingredient	CAS Number	Percent	Hazardous Chemical
Caffeine	58-08-2	>99%	No

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.

If inhaled:

If fumes or combustion products are inhaled remove from contaminated area. Lay patient down. Keep warm and rested. Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures. Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary. Transport to hospital, or doctor.

In case of skin contact:

If skin or hair contact occurs: Flush skin and hair with running water (and soap if available). Seek medical attention in event of irritation.

In case of eye contact:

If this product comes in contact with the eyes: Wash out immediately with fresh running water. Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids. Seek medical attention without delay; if pain persists or recurs seek medical attention. Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.

In case of ingestion:

IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY. For advice, contact a Poisons Information Centre or a doctor. Urgent hospital treatment is likely to be needed. In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition. If the services of a medical officer or medical doctor are readily available, the patient should be placed in his/her care and a copy of the MSDS should be provided. Further action will be the responsibility of the medical specialist.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically: For caffeine intoxication: If caffeine has been ingested within 4 hours in amount over 15mg/kg, removal from stomach by Ipecac syrup or gastric lavage is recommended. Activated charcoal is probably useful within first 4 hour. Magnesium sulphate cathartic may be useful.

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable (and unsuitable) extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder. For this substance/mixture no limitations of extinguishing agents are given.

5.2 Specific hazards arising from the substance or mixture

Carbon oxides. Nitrogen oxides (NO_x). Combustible. Development of hazardous combustion gases or vapors possible in the event of fire.

5.3 Special protective equipment and precautions for firefighters

Wear full body protective clothing with breathing apparatus. Prevent, by any means available, spillage from entering drains or water course. Use fire fighting procedures suitable for surrounding area.

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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Clean up waste regularly and abnormal spills immediately. Avoid breathing dust and contact with skin and eyes. Wear protective clothing, gloves, safety glasses and dust respirator. Use dry clean up procedures and avoid generating dust. Clear area of personnel and move upwind. Alert Fire Brigade and tell them location and nature of hazard. Wear full body protective clothing with breathing apparatus. Prevent, by any means available, spillage from entering drains or water course.

6.2 Environmental precautions

Prevent, by any means available, spillage from entering drains or water course.

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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid all personal contact, including inhalation. Wear protective clothing when risk of exposure occurs. Use in a well-ventilated area. Prevent concentration in hollows and sumps.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. See Section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Store in original containers. Keep containers securely sealed. Store in a cool, dry, well-ventilated area. Store away from incompatible materials and foodstuff containers.

SECTION 8. Exposure controls/personal protection

8.1 Occupational exposure limits

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance. Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

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). Use chemical safety goggles and/or full face shield where dusting or splashing of solutions is possible. Maintain eye wash fountain and quick-drench facilities in work area.

Skin and body protection

Wear impervious protective clothing, including boots, gloves, lab coat, apron or coveralls, as appropriate, to prevent skin contact.

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. For conditions of use where exposure to the dust or mist is apparent, a half-face dust/mist respirator may be worn. For emergencies or instances where the exposure levels are not known, use a full-face positive-pressure, air-supplied respirator. WARNING: Air-purifying respirators do not protect workers in oxygen-deficient atmospheres.

Control of environmental exposure

Do not let product enter into drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical State	Solid.
Appearance	Crystalline powder. Colorless.
Odor	Odorless.
Odor Thresh	Not applicable.
pH	6.9 [Neutral.]
Melting Point/Range	234 - 236.5 °C (453 - 457.7 °F) - lit.
Boiling Point/Range	No data available.
Flash Point	No data available.
Evaporation Rate	No data available.
Flammability (solid, gas)	No data available.
Flammability or explosive limit	Upper : No data available. Lower : No data available.
Vapor Pressure	No data available
Vapor Density	No data available.
Density	1.23 g/cm ³ at 18 °C (64 °F)
Solubility	Soluble in hot water, soluble in chloroform.
Partition coefficient; n-octanol/water	No data available
Autoignition Temp	No data available.
Decomposition Temp	1.23 g/cm ³ at 18 °C (64 °F)
Viscosity	Soluble in hot water, soluble in chloroform.
Molecular Formula	C ₈ H ₁₀ N ₄ O ₂
Molecular Weight	194.19
VOC Content(%)	No data available.
Oxidizing properties	None.

9.2 Other safety information

No data available.

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

Avoid strong acid & bases. Avoid the reaction with oxidizing agents.

10.5 Incompatible materials

No information available.

10.6 Hazardous decomposition products

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 - aerosol

(OECD Test Guideline 403)
LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)
No data available

Skin corrosion/irritation

No skin irritation.

Serious eye damage/eye irritation

No eye irritation.

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse. Result: negative

Germ cell mutagenicity

Not mutagenic in AMES Test, in vitro mammalian cell gene mutation test or chromosome aberration test in vitro.

Carcinogenicity

IARC: No ingredient 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 ingredient 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.

Chronic effects

On the basis, primarily, of animal experiments, concern has been expressed by at least one classification body that the material may produce carcinogenic or mutagenic effects; in respect of the available information, however, there presently exists inadequate data for making a satisfactory assessment. Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems. Long term exposure to high dust concentrations may cause changes in lung function (i.e. pneumoconiosis) caused by particles less than 0.5 micron penetrating and remaining in the lung. A prime symptom is breathlessness.

11.2 Additional information

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.

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

aerobic - Exposure time 22 d. Result: 90 - 100 % - Readily biodegradable.

12.3 Bioaccumulative Potential

No information 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 Endocrine disrupting properties

No information available.

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

13.1 Waste Disposal Methods

Product

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

<u>DOT</u>	Not dangerous goods.
<u>IMDG</u>	Not dangerous goods.
<u>IATA</u>	Not dangerous goods.

SECTION 15: Regulatory information

SARA 302 Components

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

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.

SECTION 16: Other information

Issue Date 06/06/2023
Revision Date 08/29/2023

Disclaimer:

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.