

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.
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1.3 Details of the supplier of the safety data sheet

Company	Lab Alley, LLC 12501 Pauls Valley Road Austin, Texas 78737 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 Oral Toxicity	Category 4
Short-term (Acute) Aquatic Hazard	Category 3

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Warning

Hazard statements

Harmful if swallowed.
Harmful to aquatic life.

Precautionary statements

Prevention: Wash skin thoroughly after handling. Do not eat, drink or smoke when using this product. Avoid release to the environment.

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

Disposal: Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

None identified.

SECTION 3: Composition/information on ingredients

3.1 Components

Chemical name	Common name and synonyms	CAS number	Concentration
Caffeine	1,3,7-trimethylxanthine; 1,3,7-trimethylpurine-2,6-dione	58-08-2	> 99%

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

If inhaled

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

In case of skin contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

In case of eye contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

If swallowed

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

4.2 Most important symptoms and effects, both acute and delayed

None reasonably foreseeable.

4.3 Indication of any immediate medical attention and special treatment needed

If symptoms persist, call a physician. Treat symptomatically.

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media Water spray, Carbon dioxide (CO₂), dry chemical, alcohol-resistant foam.

Unsuitable extinguishing media For this substance/mixture, no limitations of extinguishing agents are given.

5.2 Specific hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors. Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products: Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x).

5.3 Special protective equipment and precautions for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

5.4 Further information

Flash Point No information available.

Autoignition Temperature No information available.

Explosion limits

Upper No data available.

Lower No data available.

Sensitivity to Mechanical Impact No information available.

Sensitivity to Static Discharge No information available.

NFPA

Health	Flammability	Instability	Physical hazards
2	1	0	N/A

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.

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. Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

See Section 13 for disposal.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Precautions on 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.

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.

Incompatibilities

Strong oxidizing agents.

SECTION 8: Exposure controls/personal protection

8.1 Occupational exposure limits

This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

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

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Body Protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

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 powder
Appearance	Colorless
Odor	Odorless
Odor Threshold	No information available
pH	6.9
Melting Point/Range	234 - 236.5 °C (453 - 457.7 °F)
Boiling Point/Range	No information available
Evaporation Rate	Not applicable
Flammability (solid)	No information available
Flammability or explosive limit	No data available
Upper	
Lower	
Vapor Pressure	No information available
Vapor Density	Not applicable

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 information available
Decomposition Temp	No information available
Viscosity	Not applicable
Molecular Formula	C ₈ H ₁₀ N ₄ O ₂
Molecular Weight	194.19 g/mol
VOC Content(%)	No information available
Oxidizing properties	No information available

9.2 Other safety information

No information 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 acids and bases. Avoid reaction with oxidizing agents.

10.5 Incompatible materials

Strong oxidizing agents.

10.6 Hazardous decomposition products

Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x).

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Product Information, Component Information

Acute toxicity

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Caffeine	367.7 mg/kg (Rat)	> 2000 mg/kg (Rat)	4.94 mg/L/4h (Rat)

Skin corrosion/irritation

No information available.

Serious eye damage/eye irritation

No information available.

Respiratory or skin sensitization

No information available.

Germ cell mutagenicity

Not mutagenic in AMES Test.

Carcinogenicity

Component	CAS	IARC	NTP	ACGIH	OSHA	Mexico
Caffeine	58-08-2	Not listed	Not listed	Not listed	Not listed	Not listed

Specific target organ toxicity - single exposure

None known.

Specific target organ toxicity - repeated exposure

None known.

Reproductive toxicity

No information available.

Chronic effects

No information available.

11.2 Additional Information

The toxicological properties have not been fully investigated.

SECTION 12: Ecological information

12.1 Toxicity

Product		Species	Test Results
Caffeine	LC50	Freshwater Fish (Pimephales promelas)	151 mg/L, 96h flow-through

12.2 Persistence and degradability

Persistence is unlikely.

12.3 Bio accumulative potential

No information available.

12.4 Mobility in soil

Likely mobile in the environment due to its water solubility.

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

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

SECTION 14: Transport information

DOT (US) Not regulated.

IMDG Not regulated.

IATA Not regulated.

SECTION 15: Regulatory information

US federal regulations This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not applicable.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not regulated.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous

Acute Health Hazard, Chronic Health Hazard.

SARA 313 (TRI reporting)

Not regulated.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act

Not regulated.

FEMA Priority Substances Respiratory Health and Safety in the Flavor Manufacturing Workplace

Not listed.

US state regulations

US. Massachusetts RTK - Substance List

Not listed.

US. New Jersey Worker and Community Right-to-Know Act

Not listed.

US. Pennsylvania Worker and Community Right-to-Know Law

Not listed.

California Proposition 65

Not listed.

SECTION 16: Other information

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SECTION 17: 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.