

Material Safety Data Sheet Caffeine Anhydrous USP

1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

Chemical Name: Caffeine Anhydrous USP

Synonyms: 1,3,7-trimethylxanthine; 3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione, Trimethyl-1,3,7-dioxo-2,6-purine.

Chemical Formula: C₈-H₁₀-N₄-O₂

Application: Laboratory and Research.

Distributed By:
Ingredient Depot

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Preparation date of MSDS: 25 October 2018

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2. COMPOSITION/INFORMATION ON INGREDIENTS

COMPOSITION

Ingredients	Percentage by weight	LD50s Route & Species:
Caffeine Anhydrous CAS#: 58-08-2	100	Oral LD50 (Mouse) 127 mg/kg Oral LD50 (Rat) 192 mg/kg Oral LD50 (Rabbitt) 224 mg/kg

Notes: No additional remark.

3. HAZARDS IDENTIFICATION

Potential Acute Health Effects: Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation. Severe over-exposure can result in death.

Potential Chronic Health Effects: CARCINOGENIC EFFECTS: 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECT: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to heart, gastrointestinal tract, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure to a highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

4. FIRST AID MEASURES

Eye Contact: Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention.

Skin Contact: In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention

Serious Skin Contact: Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Serious Inhalation: Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. Seek medical attention.

Ingestion: If swallowed, do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Serious Ingestion: Not available.

5. FIRE FIGHTING MEASURES

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: Not available.

Flash Points: CLOSED CUP: Higher than 93.3°C (200°F).

Flammable Limits: Not available.

Products of Combustion: These products are carbon oxides (CO, CO₂), nitrogen oxides (NO, NO₂...).

Fire Hazards in Presence of Various Substances:

Slightly flammable to flammable in presence of open flames and sparks, of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:

Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:

SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

6. ACCIDENTAL RELEASE MEASURES

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill: Poisonous solid. Stop leak if without risk. Do not get water inside container. Do not touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal.

7. HANDLING AND STORAGE

Precautions: Keep locked up.. Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Engineering Controls: 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 Protection: Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill: Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical State and Appearance: Solid. (Crystalline solid).

Odour: Odourless.

Taste: Bitter.

Molecular Weight: 194.2 g/mole.

Color: White.

pH (1% soln/water): 6.9 [Neutral].

Boiling Point: Not available.

Melting Point: 238 °C / 460.4 °F

Critical Temperature: Not available.

Specific Gravity: 1.23 (Water = 1).

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: The product is equally soluble in oil and water; $\log(\text{oil/water}) = -0.1$.

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether.

Solubility: Soluble in hot water. Partially soluble in cold water, acetone. Very slightly soluble in diethyl ether. Freely soluble in pyrrole; in tetrahydrofuran containing about 4% water. Soluble in pyridine, ethyl acetate. Partially soluble in alcohol. Slightly soluble in petroleum ether. Solubility in water is increased by alkali benzoates, cinnamates, citrates or salicylates.

10. STABILITY AND REACTIVITY

Chemical Stability: Stable.

Instability Temperature: Not available.

Conditions to Avoid: Moisture. Extreme heat.

Materials to Avoid: Strong acids. Strong alkalis. Strong oxidizers.

Corrosivity: Non-corrosive in presence of glass

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

11. TOXICOLOGICAL INFORMATION

Routes of Entry: Inhalation. Ingestion.

Chronic Effects on Humans: CARCINOGENIC EFFECTS: 3 (Not classifiable for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. May cause damage to the following organs: heart, gastrointestinal tract, central nervous system (CNS).

Other Toxic Effects on Humans: Hazardous in case of skin contact (irritant), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: LDL [Human] - Route: Oral; Dose: 192mg/kg LDL [Woman] - Route: Oral; Dose: 400 mg/kg LDL [Child] - Route: Oral; Dose: 320 mg/kg.

Special Remarks on Chronic Effects on Humans: May cause adverse reproductive effects (fetotoxicity, maternal (parnutrition) and birth defects. May affect genetic material (mutagenic). May cause cancer (tumorigenic) based on animal data.

Special Remarks on other Toxic Effects on Humans: Acute Potential Health Effects: Skin: May cause skin irritation. Eyes: Dust may cause mechanical irritation. Inhalation: May cause respiratory tract irritation. Ingestion: Harmful if swallowed in large amounts. May cause gastrointestinal (digestive) tract irritation with epigastric pain, abdominal cramps, nausea, vomiting and diarrhea. Affects metabolism and cardiovascular system with symptoms including increase in metabolism, flushing, palpitations, rapid heart rate, dysrhythmias, hypotension, blood pressure elevation and weight loss, metabolic acidosis. May affect brain and behavior/central nervous system. Symptoms may include nervousness, anxiety, restlessness, insomnia, dizziness, tremor, seizures, convulsions, hallucinations, somnolence, toxic psychosis, tremors, convulsions, ataxia. May also affect blood, respiration (hyperventilation), and urinary system (mild increase in urinary volume and urinary sodium excretion), and may directly produce hypokalemia. Chronic Potential Health Effects: May cause cancer (tumorigen) based on animal studies. May cause reproductive and fetal effects. May cause digestive tract disturbances (increased gastric acid, and pepsin secretion and a decrease in lower esophageal sphincter pressure), cardiovascular disturbances. Since it is a CNS stimulant, it may also affect the Central Nervous System (CNS).

12. ECOLOGICAL INFORMATION

Ecotoxicological Information: Not available.

BOD5 and COD: Not available.

Products of Biodegradation: Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Waste must be disposed of in accordance with federal, state and local environmental control regulations.

14. TRANSPORT INFORMATION

DOT (U.S.):

DOT Shipping Name: Not Regulated.

DOT Hazardous Class: Not Applicable.

DOT UN Number: Not Applicable.

DOT Packing Group: Not Applicable.

DOT Reportable Quantity (lbs): Not Applicable.

Notes: No additional remark.

Marine Pollutant: No.

ICAO/IATA:

IATA Proper Shipping Name: Not Regulated.

IATA Hazard Class: Not Applicable.

UN Number: Not Applicable.

Packing Group: Not Applicable.

IATA Label: Not Applicable.

IATA Remarks: No additional remark.

IMDG:

IMDG Proper Shipping Name: Not Regulated.

Hazard Class: Not Applicable.

UN Number: Not Applicable.

Packing Group: Not Applicable.

Marine Pollutant: No.

IMDG Label: Not Applicable.

Remarks: No additional remark.

TDG (Canada):

TDG Proper Shipping Name: Not Regulated.

Hazard Class: Not Applicable.

UN Number: Not Applicable.

Packing Group: Not Applicable.

Note: No additional remark.

Marine Pollutant: No.

15. REGULATORY INFORMATION

WHMIS (Canada): Not controlled under WHMIS (Canada). Does not have a WHMIS classification.

U.S. United-States:

Federal and State Regulations: TSCA 8(b) inventory: Caffeine.

Other Classifications:

DSCL (EEC): R22- Harmful if swallowed. R40- Possible risks of irreversible effects. R63- Possible risk of harm to the unborn child. S2- Keep out of the reach of children.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 1

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 1

Reactivity: 0

Specific Hazard:

Protective Equipment:

Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Splash goggles.

16. OTHER INFORMATION

Additional Information:

This product has been classified in accordance with the hazard criteria of the Canadian Controlled Products Regulations (CPR) and the MSDS contains all the information required by the CPR.

Disclaimer:

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*****END OF MSDS*****