Section 1 - Product and Company Information

Product Name: Caffeine, anhydrous
Product Number: C7731
Brand: Sigma-Aldrich
Company: Sigma-Aldrich
Street Address: 3050 Spruce Street
City, State, Zip, Country: SAINT LOUIS, MO 63103 US
Technical Phone: 800-352-6800
Fax: 800-325-6052
Emergency Phone: 314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name: Caffeine
CAS #: 58-09-2
SARA 313: No
EC No: 200-362-1
Annex I Index Number: 613-086-03-5

Formula: C8H10N4O2
Synonyms: Anhydrous caffeine, Caftan, Caffina (Italian), Coffein (German), Coffeine, Coffeïnum, 3,7-Dihydroxy-1,3,7-trimethyl-1H-purine-2,6-dione, Edelkaffe C, Guarana, Koffein (Czech), Koffein (German), Methyldopa, NCI-C02732, NC-Dox. Organex: 1H-Purine-2,8-dione, 3,7-dihydro-1,3,7-trimethyl-, Theobroma, 1,3,7-Trimethyl-1H-purine-2,6-dione, 1,3,7-Trimethylxantidine, Xanthyl, 1.3,7-Trimethylxanthine

Section 3 - Hazards Identification

Emergency Overview
Toxic.
In case of contact, immediately flush eyes or skin with copious amounts of water for at least 15 minutes while removing contaminated clothing and shoes.

NFPA Rating
Health: 2
Flammability: 0
Reactivity: 0

Molecular Weight: 194.19 AMU
pH: N/A
BP/BP Range: N/A
MP/MP Range: 232 °C
Freezing Point: N/A

Section 4 - First Aid Measures

Immediate Treatment - Work Site
In case of contact, immediately flush eyes or skin with copious amounts of water for at least 15 minutes while removing contaminated clothing and shoes.

Inhalation Exposure
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.

Section 5 - Fire Fighting Measures

Autoignition Temp: N/A
Extinguishing Media
Suitable: Carbon dioxide

Firefighting
Protective Equipment
Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s)
Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

Procedure(s) of Personal Precaution(s)
Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.
Method(s) for Cleaning Up
Sweep up, place in a bag and hold for waste disposal. Avoid raising dust.

Section 7 - Handling and Storage

Handling
User Exposure
Do not breathe dust. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.
Storage
Suitable: Keep tightly closed. Store in a cool dry place.

Section 8 - Exposure Controls / PPE

Engineering Controls
Use only in a chemical fume hood. Safety shower and eye bath.

Personal Protective Equipment
Other
Wear appropriate government approved respirator, chemical-resistant gloves, safety goggles, other protective clothing.

General Hygiene Measures
Wash contaminated clothing before reuse. Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance
Color: White
Form: Powder

Molecular Weight: 194.19 AMU
Section 10 - Stability and Reactivity

Stability
Stable.

Materials to Avoid
Strong oxidizing agents.

Hazardous Decomposition Products
Carbon monoxide, carbon dioxide, and nitrogen oxides.

Hazardous Polymerization
Will not occur.

Section 11 - Toxicological Information

Route of Exposure
Skin Absorption
May be harmful if absorbed through the skin.

Inhalation
May be harmful if inhaled.

Ingestion
May be harmful if swallowed.

Target Organ(s) or System(s)
Central nervous system. Heart.

Toxicity Data

Oral - Woman: 400 mg/kg (LD50)
Remarks: Behavioral/Convulsions or effect on seizure threshold.
Cardiac/Other changes. Skin and Appendages: Other. Sweating.

Oral - Human: 192 mg/kg (LD50)

Oral - Child: 320 mg/kg (LD50)
Remarks: Behavioral/Convulsions or effect on seizure threshold.
Lungs, Thorax, or Respiratory/Cyanosis.

Oral - Woman: 1000 mg/kg (LD50)
Remarks: Gastrointestinal Nausea or vomiting.

Intravenous - Woman: 57 MG/KG (LD50)
Remarks: Behavioral/Convulsions or effect on seizure threshold.
Vascular/BP elevation not characteristic in autonomic section.

Oral - Rat: 102 mg/kg (LD50)
Remarks: Brain and Coverings Other degenerative changes.

Intrapertoneal - Rat: 240 MG/KG (LD50)

Subcutaneous - Rat: 170 MG/KG (LD50)

Intravenous - Rat: 105 MG/KG (LD50)
Remarks: Lungs, Thorax, or Respiratory Acute pulmonary edema.
Kidney, Ureter, Bladder/Structural or functional changes in ureter.

Rectal - Rat: 300 MG/KG (LD50)

Oral - Mouse: 127 mg/kg (LD50)
Remarks: Gastrointestinal Hypomotility, diarrhea.

Intrapertoneal - Mouse: 168 MG/KG (LD50)
Remarks: Behavioral Change in motor activity (specific assay).
Behavioral Depression. Kidney, Ureter, Bladder/Urinary tract volume increased.

Subcutaneous - Mouse: 242 MG/KG (LD50)

Intravenous - Mouse: 62 MG/KG (LD50)
Remarks: Behavioral/Convulsions or effect on seizure threshold.
Lungs, Thorax, or Respiratory/Dyspnea.

Oral - Dog: 140 mg/kg (LD50)

Subcutaneous - Dog: 100 MG/KG (LD50)

Oral - Rabbit: 224 mg/kg (LD50)
Remarks: Gastrointestinal Hypomotility, diarrhea.

Intravenous - Rabbit: 56 MG/KG (LD50)

Oral - Guinea pig: 230 mg/kg (LD50)
Remarks: Behavioral/Convulsions or effect on seizure threshold.
Lungs, Thorax, or Respiratory/Respiratory depression.

Oral - Hamster: 230 mg/kg (LD50)
Remarks: Gastrointestinal Hypomotility, diarrhea.

Oral - Bird (w/d): 316 mg/kg (LD50)

Chronic Exposure - Carcinogen
Mouse - Oral: 30800 MG/KG 44W C

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### Chronic Exposure - Teratogen

**Species**
- **Woman**: 6750 MG/KG
- **Rat**: 200 MG/KG
- **Mouse**: 350 MG/KG
- **Mouse**: 1650 MG/KG
- **Mouse**: 2691 MG/KG
- **Mouse**: 250 MG/KG
- **Mouse**: 200 MG/KG
- **Mouse**: 150 MG/KG
- **Hamster**: 300 MG/KG
- **Hamster**: 125 MG/L
- **Hamster**: 1 MMOL/L
- **Hamster**: 2 MMOL/L
- **Hamster**: 10 MMOL/L
- **Hamster**: 25 MMOL/L
- **Hamster**: 1 MML/L
- **Hamster**: 2 MML/L
- **Hamster**: 4 MML/L
- **Hamster**: 300 MMOL/L
- **Chicken**: 25 MMOL/L
- **Mammal**: 100 MMOL/L

**Route of Application**
- Oral
- Intraperitoneal
- Intraocular
- Intravenous

**Exposure Time**
- (1-3W PREG)
- (13-14D PREG)
- (15-21D PREG)
- (1-10D PREG)
- (11D PREG)
- (6-16D PREG)
- (5-18D PREG)
- (10D PREG)
- (12D PREG)
- (6W PREG/12D PREG)
- (1-5W PREG)
- (1-9D PREG)
- (1-22D PREG)

**Specific Developmental Abnormalities**
- Craniofacial (including nose and tongue)
- Musculoskeletal system
- Central nervous system
- Craniofacial (including nose and tongue)
- Musculoskeletal system
- Craniofacial (including nose and tongue)
- Musculoskeletal system
- Craniofacial (including nose and tongue)
- Musculoskeletal system
- Craniofacial (including nose and tongue)
- Musculoskeletal system

**Related Information**
- **Note**: Specific Developmental Abnormalities: Craniofacial (including nose and tongue).
- **Note**: Specific Developmental Abnormalities: Musculoskeletal system.

### Chronic Exposure - Mutagen

**Species**
- **Human**: 750 UMO/L
- **Human**: 1 MMOL/L
- **Human**: 4 MMOL/L
- **Human**: 1 MMOL/L
- **Human**: 2800 UMO/L
- **Human**: 100 UCL/L
- **Human**: 50 MMOL/L
- **Human**: 50 MG/KG
- **Human**: 100 MG/KG
- **Mouse**: 100 MG/L
- **Mouse**: 10 MG/L
- **Mouse**: 7 MG/L
- **Mouse**: 50 MG/KG
- **Mouse**: 5 MMOL/L
- **Mouse**: 5 MG/L
- **Mouse**: 14 MG/KG
- **Mouse**: 50 MG/KG
- **Mouse**: 100 MG/L
- **Mouse**: 50 MG/KG
- **Mouse**: 5 MMOL/L
- **Mouse**: 5 MG/L
- **Hamster**: 300 MG/KG
- **Hamster**: 25 MMOL/L
- **Hamster**: 4 MML/L
- **Hamster**: 2 MML/L
- **Hamster**: 10 MMOL/L
- **Chicken**: 25 MMOL/L
- **Mammal**: 100 MMOL/L
- **Mammal**: 10 MMOL/L

**Route of Application**
- Oral
- Intraperitoneal
- Intravenous
- Oral
- Oral
- Oral
- Oral
- Oral
- Oral
- Oral
- Intraperitoneal
- Intraperitoneal
- Intraperitoneal
- Intravenous
- Intravenous
- Oral
- Oral
- Oral
- Oral
- Oral
- Oral
- Oral

**Exposure Time**
- (1-5W PREG)
- (1-9D PREG)
- (1-22D PREG)

**Cell Type**
- fibroblast
- leucocyte
- lymphocyte
- leucocyte
- lymphocyte
- leucocyte
- lymphocyte
- fibroblast
- leucocyte
- lymphocyte
- leucocyte
- fibroblast
- lymphocyte
- fibroblast

**Mutation Test**
- DNA repair
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition
- DNA inhibition

**Related Information**
- **Note**: Specific Developmental Abnormalities: Craniofacial (including nose and tongue).
- **Note**: Specific Developmental Abnormalities: Musculoskeletal system.

### Chronic Exposure - Reproductive Hazard

**Species**
- **Woman**: 1692 MG/KG
- **Rat**: 627 MG/KG

**Route of Application**
- Oral

**Exposure Time**
- (1-5W PREG)
- (1-22D PREG)

**Related Information**
- **Note**: Specific Developmental Abnormalities: Craniofacial (including nose and tongue).
- **Note**: Specific Developmental Abnormalities: Musculoskeletal system.
Section 15 - Regulatory Information

EU Directives Classification
Symbol of Danger: Xn
Indication of Danger
Harmful
Risk Statements
R: 22
Harmful if swallowed.

US Classification and Label Text
Indication of Danger
Toxic
Risk Statements
Toxic if swallowed. Irritating to eyes, respiratory system and skin. Limited evidence of a carcinogenic effect.

Safety Statements
In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Wear suitable protective clothing, gloves, and eye/face protection. Do not breathe dust.

US Statements
Target organ(s): Central nervous system. Heart.

United States Regulatory Information
SARA Listed: No

TSCA Inventory Item: Yes

Canada Regulatory Information
WHMIS Classification
This product has been classified in accordance with the hazard criteria of the CPR, and the MDSD contains all the information required by the CPR.

DSL: Yes
NDSSL: No

Section 16 - Other Information

Disclaimer
For R&D or manufacturing use. Not for prescription compound or other uses.

Warranty
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. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2007 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.