4/26/07

SIGMA-ALDRICH

Material Safety Data Sheet

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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: 800-325-5832 **Emergency Phone:** 314-776-6555
Fax: 800-325-5052

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313	EC no	Annex I Index Number
CAFFEINE MEETS USP TESTING SPECS.	58-08-2	No	200-362-1	613-086-00-5

Formula C8H10N4O2
Synonyms Anhydrous caffeine, Caffein, Caffeina (Italian), Coffein (German), Coffeine, Coffeinum, 3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione, Eldiatric C, Guaranine, Kofein (Czech), Koffein (German), Methyltheobromide, NCI-C02733, NO-Doz, Organex, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-, Thein, Theine, Theobromine, 1-methyl-, Theophylline, 7-methyl, 1,3,7-Trimethyl-2,6-dioxopurine, 1,3,7-Trimethylxanthine, Xanthine, 1,3,7-trimethyl

Section 3 - Hazards Identification

Emergency Overview
Toxic.
Toxic if swallowed. Irritating to eyes, respiratory system and skin. Limited evidence of a carcinogenic effect.
Target organ(s): Central nervous system. Heart.

HMIS Rating
Health: 2 Flammability: 0 Reactivity: 0

NFPA Rating
Flammability: 0 Reactivity: 0

For additional information on toxicity, please refer to Section 11.

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.

Methods 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	Form
White	Powder

Molecular Weight: 194.19 AMU

pH N/A
BP/BP Range N/A
MP/MP Range 232 °C
Freezing Point N/A

Vapor Pressure	N/A
Vapor Density	N/A
Saturated Vapor Conc.	N/A
SG/Density	N/A
Bulk Density	N/A
Odor Threshold	N/A
Volatile%	N/A
VOC Content	N/A
Water Content	N/A
Solvent Content	N/A
Evaporation Rate	N/A
Viscosity	N/A
Partition Coefficient	N/A
Decomposition Temp.	N/A
Flash Point °F	N/A
Flash Point °C	N/A
Explosion Limits	N/A
Flammability	N/A
Autoignition Temp	N/A
Solubility	N/A

N/A = not available

Section 10 - Stability and Reactivity

Stability

Stable

Stable.

Materials to Avoid

Strong oxidizing agents.

Hazardous Decomposition Products

Hazardous Decomposition Products

Carbon monoxide, carbon dioxide, and nitrogen oxides.

Hazardous Polymerization

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

Harmful if swallowed.

Multiple Routes

Causes eye and skin irritation.

Target Organ(s) or System(s)

Central nervous system. Heart.

Signs and Symptoms of Exposure

Overexposure by ingestion may result in nervousness, tremors, and insomnia. Headache, dizziness, drowsiness, incoordination, slowed reaction time, slurred speech, giddiness and unconsciousness. Lethargy and convulsions. Nausea, vomiting, diarrhea. Ataxia. CNS stimulation. Convulsions. Prolonged or repeated exposure can lead to habituation or addiction. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

RTECS Number: EV6475000

Toxicity Data

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

Oral - Human: 192 mg/kg (LDLO)

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

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

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

Oral - Rat: 192 mg/kg (LD50)
Remarks: Brain and Coverings:Other degenerative changes.
Behavioral:Withdrawal.
Kidney, Ureter, Bladder:Interstitial nephritis.

Intraperitoneal - Rat: 240 MG/KG (LD50)

Subcutaneous - Rat: 170 MG/KG (LD50)

Intravenous - Rat: 105 MG/KG (LD50)
Remarks: Lungs, Thorax, or Respiration: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:Hypermotility, diarrhea.

Intraperitoneal - Mouse: 168 MG/KG (LD50)
Remarks: Behavioral:Change in motor activity (specific assay).
Behavioral:Aggression.
Kidney, Ureter, Bladder:Urine 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 Respiration:Dyspnea.

Oral - Dog: 140 mg/kg (LD50)

Subcutaneous - Dog: 100 MG/KG (LD50)

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

Intravenous - Rabbit: 58 MG/KG (LD50)

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

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

Oral - Bird (wild): 316 mg/kg (LD50)

Chronic Exposure - Carcinogen

Mouse - Oral: 30800 MG/KG 44W C
Result: Tumorigenic:Carcinogenic by RTECS criteria. Skin and Appendages: Other: Tumors. Tumorigenic:Increased incidence of tumors in susceptible strains.

IARC Carcinogen List

Rating
Group 3

Chronic Exposure - Teratogen

Species	*Dose*	*Route of Application*	*Exposure Time*
Woman	6750 MG/KG	Oral	(1-39W PREG)
	Result:Specific Developmental Abnormalities: Craniofacial (including nose and tongue). Specific Developmental Abnormalities: Musculoskeletal system.		
Rat	200 MG/KG	Oral	(13-14D PREG)
	Result:Effects on Embryo or Fetus: Extra embryonic structures (e.g., placenta, umbilical cord). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).		
Rat	1750 MG/KG	Oral	(15-21D PREG)
	Result:Specific Developmental Abnormalities: Blood and lymphatic system (including spleen and marrow). Specific Developmental Abnormalities: Homeostasis		
Rat	114 MG/KG	Oral	(1-19D PREG)
	Result:Specific Developmental Abnormalities: Musculoskeletal system.		
Rat	120 MG/KG	Oral	(12D PREG)
	Result:Effects on Embryo or Fetus: Maternal-fetal exchange.		
Rat	75 MG/KG	Intraperitoneal	(12D PREG)
	Result:Specific Developmental Abnormalities: Central nervous system. Specific Developmental Abnormalities: Eye, ear.		
Rat	37500 UG/KG	Intravenous	(11D PREG)
	Result:Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).		
Rat	25 MG/KG	Intravenous	(6D PREG)
	Result:Specific Developmental Abnormalities: Musculoskeletal system.		
Rat	113 MG/KG	Intravenous	(11D PREG)
	Result:Specific Developmental Abnormalities: Musculoskeletal system.		
Mouse	350 MG/KG	Oral	(8D PREG)
	Result:Specific Developmental Abnormalities: Musculoskeletal system.		
Mouse	1650 MG/KG	Oral	(6-16D PREG)
	Result:Specific Developmental Abnormalities: Central nervous system. Specific Developmental Abnormalities: Craniofacial (including nose and tongue). Specific Developmental Abnormalities: Musculoskeletal system.		
Mouse	2691 MG/KG	Oral	(5-18D PREG)
	Result:Specific Developmental Abnormalities: Other developmental abnormalities.		
Mouse	250 MG/KG	Intraperitoneal	(10D PREG)
	Result:Effects on Embryo or Fetus: Fetal death.		
Mouse	200 MG/KG	Intraperitoneal	(12D PREG)
	Result:Specific Developmental Abnormalities: Musculoskeletal system. Specific Developmental Abnormalities: Other developmental abnormalities.		
Mouse	150 MG/KG	Subcutaneous	(13D PREG)
	Result:Specific Developmental Abnormalities: Craniofacial (including nose and tongue). Specific Developmental Abnormalities: Musculoskeletal system. Specific Developmental Abnormalities: Other developmental abnormalities.		
Mouse	400 MG/KG	Subcutaneous	(13D PREG)
	Result:Specific Developmental Abnormalities: Gastrointestinal system.		
Mouse	200 MG/KG	Intravenous	(13D PREG)
	Result:Specific Developmental Abnormalities: Craniofacial (including nose and tongue). Specific Developmental Abnormalities: Other developmental abnormalities.		
Mouse	408 MG/KG	Multiple	(9W PRE/12D PREG)
	Result:Specific Developmental Abnormalities: Skin and skin appendages.		

Chronic Exposure - Mutagen

Species	*Dose*			*Cell Type*	*Mutation test*
Human	750 UMOL/L			fibroblast	DNA repair
Human	1 MMOL/L			Other cell types	Unscheduled DNA synthesis
Human	1 MMOL/L			HeLa cell	DNA inhibition
Human	4 MMOL/L			Other cell types	DNA inhibition
Human	1 MMOL/L			lymphocyte	Other mutation test systems
Human	100 MG/L			leukocyte	Cytogenetic analysis
Human	2600 UMOL/L		24H	fibroblast	Cytogenetic analysis
Human	100 UG/L		24H	lymphocyte	Cytogenetic analysis
Human	50 PPM		24H	Embryo	Cytogenetic analysis
Human	500 MG/L			HeLa cell	Cytogenetic analysis
Human	1 MMOL/L			lymphocyte	Sister chromatid exchange
Rat	10 MMOL/L			kidney	Micronucleus test
Rat	320 UG/PLATE			Embryo	Morphological transformation.
Rat	200 UMOL/L			Other cell types	DNA inhibition
Mouse	7 MMOL/L			Embryo	Micronucleus test
Mouse	100 MG/KG	Oral			Micronucleus test
Mouse	35 MG/KG	Intraperitoneal			specific locus test
Mouse	100 MG/KG	Intraperitoneal			DNA damage
Mouse	100 UMOL/L			leukocyte	DNA damage
Mouse	50 MG/KG	Intraperitoneal			DNA inhibition
Mouse	208 MG/KG	Oral	7D		DNA inhibition
Mouse	5 MMOL/L			lymphocyte	DNA inhibition
Mouse	5 MMOL/L			fibroblast	DNA inhibition
Mouse	50 MG/KG	Intraperitoneal			Other mutation test systems
Mouse	14 MG/KG	Oral	7D		Cytogenetic analysis
Mouse	50 MG/KG	Intravenous			Cytogenetic analysis
Mouse	7700 UMOL/L			Ascites tumor	Cytogenetic analysis
Mouse	100 MG/L			lymphocyte	Cytogenetic analysis
Mouse	50 MG/KG	Intravenous			Sister chromatid exchange
Mouse	5 GM/KG	Oral	5D		Sister chromatid exchange
Mouse	100 UMOL/L			Other cell types	Sister chromatid exchange
Mouse	2520 MG/KG	Oral	W		Dominant lethal test
Mouse	500 MG/L			lymphocyte	Mutation in mammalian somatic cells.
Mouse	150 MG/KG			Ascites tumor	Host-mediated assay
Hamster	300 MG/KG	Oral			Micronucleus test
Hamster	125 MG/L			Embryo	Morphological transformation.
Hamster	1 MMOL/L			lung	DNA inhibition
Hamster	2 MMOL/L			ovary	Cytogenetic analysis
Hamster	10 MMOL/L			lung	Cytogenetic analysis
Hamster	25 MMOL/L		2H	Other cell types	Cytogenetic analysis
Hamster	1 GM/L			fibroblast	Cytogenetic analysis
Hamster	4 MMOL/L			lung	Sister chromatid exchange
Hamster	300 MG/KG	Oral			Sister chromatid exchange
Chicken	25 MMOL/L			fibroblast	Cytogenetic analysis
Mammal	100 MMOL/L			lymphocyte	DNA damage
Mammal	10 MMOL/L			lymphocyte	DNA inhibition

Chronic Exposure - Reproductive Hazard

Species	*Dose*	*Route of Application*	*Exposure Time*
Woman	3276 MG/KG	Oral	(1-39W PREG)
	Result: Maternal Effects: Parturition. Effects on Newborn: Stillbirth.		
Woman	1092 MG/KG	Oral	(1-91D PREG)
	Result: Effects on Fertility: Abortion.		
Rat	627 MG/KG	Oral	(1-22D PREG)
	Result: Effects on Newborn: Biochemical and metabolic. Effects on Newborn: Other postnatal measures or effects.		

Rat 85 MG/KG Oral (3-19D PREG)
Result: Effects on Newborn: Behavioral. Effects on Newborn: Physical.
Rat 660 MG/KG Oral (1-22D PREG)
Result: Effects on Fertility: Female fertility index (e.g., # females pregnant per # sperm positive females; # females pregnant per # females mated). Specific Developmental Abnormalities: Urogenital system. Effects on Newborn: Weaning or lactation index (e.g., # alive at weaning per # alive at day 4).
Rat 420 MG/KG Intraperitoneal (1-21D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).
Rat 200 MG/KG Subcutaneous (4D MALE)
Result: Effects on Newborn: Viability index (e.g., # alive at day 4 per # born alive).
Mouse 1 GM/KG Oral (8-12D PREG)
Result: Effects on Newborn: Growth statistics (e.g., reduced weight gain).
Mouse 1650 MG/KG Oral (6-16D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).
Mouse 500 MG/KG Intraperitoneal (11-12D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Specific Developmental Abnormalities: Other developmental abnormalities.
Mouse 200 MG/KG Intraperitoneal (12D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus). Specific Developmental Abnormalities: Craniofacial (including nose and tongue).
Mouse 200 MG/KG Subcutaneous (12D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus). Specific Developmental Abnormalities: Craniofacial (including nose and tongue).
Mouse 150 MG/KG Subcutaneous (13D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth).
Hamster 8160 MG/KG Oral (60D MALE)
Result: Effects on Newborn: Sex ratio.

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

Appropriate Method of Disposal of Substance or Preparation
Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT
Proper Shipping Name: Alkaloids, solid, n.o.s. [or] Alkaloid salts, solid, n.o.s. [poisonous]
UN#: 1544
Class: 6.1
Packing Group: Packing Group III
Hazard Label: Toxic substances.
PIH: Not PIH

IATA
Proper Shipping Name: Alkaloids, solid, n.o.s.
IATA UN Number: 1544
Hazard Class: 6.1
Packing Group: III

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 MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: 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.