

# Material Safety Data Sheet

HAZARD WARNINGS	RISK PHRASES	PROTECTIVE CLOTHING
  	<p><b>Toxic compound, do not ingest or inhale. Avoid all contact with this material.</b>  <b>Irritating to skin, eyes, and the respiratory system.</b>  <b>CARCINOGEN. MINIMIZE EXPOSURE.</b>  <b>MUTAGEN. MINIMIZE EXPOSURE.</b></p>	   

## Section I. Chemical Product and Company Identification

Chemical Name	<b>Caffeine</b>		
Catalog Number	C2042	Supplier	TCI America 9211 N. Harborgate St. Portland OR 1-800-423-8616
Synonym	1,3,7-Trimethylxanthine		
Chemical Formula	C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>		
CAS Number	58-08-2	In case of Emergency Call	<b>Chemtrec®</b> <b>(800) 424-9300 (U.S.)</b> <b>(703) 527-3887</b> <b>(International)</b>

## Section II. Composition and Information on Ingredients

Chemical Name	CAS Number	Percent (%)	TLV/PEL	Toxicology Data
Caffeine	58-08-2	Min. 98.0 (HPLC,T)	This chemical is classified as a carcinogen. There is no acceptable exposure limit for a carcinogen. This compound is classified as a mutagen. There is no acceptable exposure limit for a mutagen.	Rat LD <sub>50</sub> (oral) 192 mg/kg Mouse LD <sub>50</sub> (oral) 168 mg/kg Rat LD <sub>50</sub> (intravenous) 105 mg/kg Rat LD <sub>50</sub> (subcutaneous) 170 mg/kg Rat LD <sub>50</sub> (intraperitoneal) 240 mg/kg

## Section III. Hazards Identification

Acute Health Effects	<p>Toxic if ingested or inhaled. Avoid prolonged contact with this material. Overexposure may result in serious illness or death.</p> <p>Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.</p> <p>Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.</p>
Chronic Health Effects	<p><b>CARCINOGENIC EFFECTS</b> : Carcinogenic by RTECS criteria.</p> <p><b>MUTAGENIC EFFECTS</b> : Not available.</p> <p><b>TERATOGENIC EFFECTS</b> : Tumorigenic Effects.</p> <p>Mouse TDLo Oral 30800 mg/kg/44 weeks continuous</p> <p>TOXIC Effects:</p> <p>Tumorigenic – Carcinogenic by RTECS criteria</p> <p>Skin and Appendages – Tumors</p> <p>Tumorigenic – Increased incidence of tumors in susceptible strains</p> <p>Rat TDLo Oral 4200 mg/kg/10 weeks continuous</p> <p>TOXIC Effects:</p> <p>Tumorigenic – Neoplastic by Rtecs criteria</p> <p>Gastrointestinal – Colon tumors</p> <p>Tumorigenic – Facilitates action of known carcinogens</p> <p><b>DEVELOPMENTAL TOXICITY</b> : Reproductive Effects.</p> <p>Rat TDLo Intraperitoneal 75 mg/kg, female 1-21 days of pregnancy</p> <p>TOXIC Effects:</p> <p>Specific Developmental Abnormalities – Central Nervous system</p> <p>Specific Developmental Abnormalities – Eye, ear</p> <p>Woman TDLo Oral 84 mg/kg, female 1-42 days of pregnancy</p> <p>TOXIC Effects:</p> <p>Effects on Fertility – Abortion</p> <p>Rat TDLo Oral 12.5 mg/kg, female multigenerations</p> <p>TOXIC Effects:</p> <p>Effects on Newborn – Growth statistics</p>

## Section IV. 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. Get medical attention.
Skin Contact	In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.
Inhalation	If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention if respiration problems do not improve.

## Ingestion

INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive.

**Section V. Fire and Explosion Data**

Flammability	May be combustible at high temperature.	Auto-Ignition	540°C (1004°F)
Flash Points	Not available.	Flammable Limits	Not available.
Combustion Products	These products are toxic carbon oxides (CO, CO <sub>2</sub> ), nitrogen oxides (NO, NO <sub>2</sub> ).		
Fire Hazards	Not available.		
Explosion Hazards	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. Consult with local fire authorities before attempting large scale fire-fighting operations.		

**Section VI. Accidental Release Measures**

Spill Cleanup Instructions	Toxic material. Irritating material. Carcinogenic material. Mutagenic material. 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 sources of ignition. Consult federal, state, and/or local authorities for assistance on disposal.
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**Section VII. Handling and Storage**

Handling and Storage Information	TOXIC. IRRITANT. CARCINOGEN. MUTAGEN. Keep locked up. Keep away from heat. Mechanical exhaust required. When not in use, tightly seal the container and store in a dry, cool place. Avoid excessive heat and light. DO NOT ingest. Do not breathe dust. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label. Treat symptomatically and supportively.
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**Section VIII. 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. Boots. Gloves. A MSHA/NIOSH approved respirator must be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product. 
Exposure Limits	This chemical is classified as a carcinogen. There is no acceptable exposure limit for a carcinogen. This compound is classified as a mutagen. There is no acceptable exposure limit for a mutagen.

**Section IX. Physical and Chemical Properties**

Physical state @ 20°C	Solid. (White, Powder)	Solubility	One gram dissolves in 46 ml water, 5.5 ml water at 80°, 1.5 ml boiling water, 66 ml alcohol, 22 ml alcohol at 60°, 50 ml acetone, 5.5 ml chloroform, 530 ml ether, 100 ml benzene, 22 ml boiling benzene. Freely soluble in pyrrole; in tetrahydrofuran containing about 4% water; also soluble in ethyl acetate; slightly in petroleum ether. Solubility in water is increased by alkali benzoates, cinnamates, citrates or salicylates.
Specific Gravity	1.23 (water=1)	Partition Coefficient	Log K <sub>ow</sub> : -0.070
Molecular Weight	194.19	Vapor Pressure	2.0 kPa (@ 89°C)
Boiling Point	Not available.	Vapor Density	Not available.
Melting Point	238°C (460.4°F)	Volatility	Not available.
Refractive Index	1.4936 (@ 25°C)	Odor	Odorless.
Critical Temperature	Not available.	Taste	Bitter.
Viscosity	Not available.		

**Section X. Stability and Reactivity Data**

Stability	This material is stable if stored under proper conditions. (See Section VII for instructions)
Conditions of Instability	Avoid excessive heat and light.
Incompatibilities	Reactive with strong oxidizing agents.

**Section XI. Toxicological Information**

RTECS Number	EV6475000
Routes of Exposure	Eye Contact. Ingestion. Inhalation.
Toxicity Data	Rat LD <sub>50</sub> (oral) 192 mg/kg Mouse LD <sub>50</sub> (oral) 168 mg/kg Rat LD <sub>50</sub> (intravenous) 105 mg/kg Rat LD <sub>50</sub> (subcutaneous) 170 mg/kg Rat LD <sub>50</sub> (intraperitoneal) 240 mg/kg
Chronic Toxic Effects	<b>CARCINOGENIC EFFECTS</b> : Carcinogenic by RTECS criteria. <b>MUTAGENIC EFFECTS</b> : Not available. <b>TERATOGENIC EFFECTS</b> : Tumorigenic Effects. Mouse TDLo Oral 30800 mg/kg/44 weeks continuous TOXIC Effects: Tumorigenic – Carcinogenic by RTECS criteria Skin and Appendages – Tumors Tumorigenic – Increased incidence of tumors in susceptible strains Rat TDLo Oral 4200 mg/kg/10 weeks continuous TOXIC Effects: Tumorigenic – Neoplastic by Rtecs criteria Gastrointestinal – Colon tumors Tumorigenic – Facilitates action of known carcinogens <b>DEVELOPMENTAL TOXICITY</b> : Reproductive Effects. Rat TDLo Intraperitoneal 75 mg/kg, female 1–21 days of pregnancy TOXIC Effects: Specific Developmental Abnormalities – Central Nervous system Specific Developmental Abnormalities – Eye, ear Woman TDLo Oral 84 mg/kg, female 1–42 days of pregnancy TOXIC Effects: Effects on Fertility – Abortion Rat TDLo Oral 12.5 mg/kg, female multigenerations TOXIC Effects: Effects on Newborn – Growth statistics
Acute Toxic Effects	Toxic if ingested or inhaled. Avoid prolonged contact with this material. Overexposure may result in serious illness or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

**Section XII. Ecological Information**

Ecotoxicity	Not available.
Environmental Fate	Caffeine's production and use as a stimulant and food additive may result in its release to the environment through various waste streams. Caffeine is found in coffee beans, tea leaves, cocoa beans, mate leaves, guarana paste, and kola nuts. If released to air, an estimated vapor pressure of 7.3X10 <sup>-9</sup> mm Hg at 25 deg C indicates caffeine will exist solely as a particulate in the atmosphere. Particulate-phase caffeine may be removed from the air by wet and dry deposition. Caffeine does not absorb light at wavelengths > 290 nm and therefore is not expected to be susceptible to direct photolysis by sunlight. If released to soil, caffeine is expected to have very high mobility based upon an estimated Koc of 22. Volatilization from water and moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 3.6X10 <sup>-11</sup> atm-cu m/mole. The pKa of caffeine is 10.4, indicating that this compound will primarily exist in the cation form in the environment and cations do not volatilize from water or moist soil surfaces and generally adsorb more strongly to organic carbon and clay than their neutral counterparts. Caffeine is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Caffeine has been reported to be readily biodegradable when incubated with sewage sludge. If released into water, caffeine is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. The estimated half-life of 0.8 days based upon river infiltration, suggests biodegradation may be an important environmental fate process in water. Occupational exposure to caffeine may occur through dermal contact with this compound at workplaces where caffeine is produced or used. Caffeine is found as an additive in many beverages and some foods and is the most common drug used in the world. The most likely route of exposure to caffeine among the general population occurs through the ingestion of beverages and food that contain caffeine, a stimulant.

**Section XIII. Disposal Considerations**

## Waste Disposal

Recycle to process, if possible. Consult your local regional authorities. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and local regulations when disposing of the substance.

**Section XIV. Transport Information**

## DOT Classification

DOT Class 6.1: Toxic material

## PIN Number

UN1544

## Proper Shipping Name

Alkaloids solids, n.o.s.

## Packing Group (PG)

III

## DOT Pictograms

**Section XV. Other Regulatory Information and Pictograms**

## TSCA Chemical Inventory (EPA)

This compound is **ON** the EPA Toxic Substances Control Act (TSCA) inventory list.

## WHMIS Classification (Canada)

CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC).  
 CLASS D-2B: Material causing other toxic effects (TOXIC).  
 On DSL

## EINECS Number (EEC)

200-362-1

## EEC Risk Statements

R23/24/25- Toxic by inhalation, in contact with skin and if swallowed.  
 R36/37/38- Irritating to eyes, respiratory system and skin.  
 R45- May cause cancer.  
 R46- May cause heritable genetic damage.

## Japanese Regulatory Data

ENCS No. 9-419

**Section XVI. Other Information****Version 1.0****Validated on 2/22/2007.****Printed 2/22/2007.****Notice to Reader**

TCI laboratory chemicals are for research purposes only and are NOT intended for use as drugs, food additives, household, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our MSDS sheets are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated MSDS sheets for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, facial mask, fume hood). For proper handling and disposal, always comply with federal, state, and local regulations.