CATO Research Chemicals Inc.
3/F,Building B,No.179 BASIGO, Guangpu Rd East,Huangpu Dist,Guangzhou
Web: www.cato-chem.com
Tel: +86-20-81960175 Fax: +86-20-81717260 E-mail: info@cato-chem.com

SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.2
Creation Date: July 15, 2019
Revision Date: August 08, 2025

SECTION 1: Identification

1.1 GHS Product identifier

Product name KFY in Methanol Certified Reference Material

1.2 Other means of identification

Product number CPRM1730
Other names 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-; Stim; No-Doz

1.3 Recommended use of the chemical and restrictions on use

Identified uses For laboratory and Industrial use only.
Uses advised against no data available

1.4 Supplier's details

Company CATO Research Chemicals Inc.
Address 3/F,Building B,No.179 BASIGO, Guangpu Rd East,Huangpu Dist,Guangzhou
Telephone +86-20-81960175

1.5 Emergency phone number

Emergency phone number +86-20-81960175
Service hours 'Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Acute toxicity - Category 4, Oral

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word Warning
Hazard statement(s) H302 Harmful if swallowed
Precautionary statement(s)
Prevention P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
Response P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
Storage none
Disposal P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
KFY in Methanol Certified Reference Material	Caffeine	58-08-2	200-362-1	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Refer for medical attention .

4.2 Most important symptoms/effects, acute and delayed

SYMPTOMS: Symptoms of exposure to this compound may include central nervous system stimulation, less drowsiness, less fatigue, more rapid and clearer flow of thought, decreased reaction time, affects on muscular coordination, accurate timing and arithmetic skills, nervousness, restlessness, insomnia, tremors and hyperesthesia. At higher doses, symptoms include focal and generalized convulsions, Cheyne-Stokes respiration, apnea of preterm infants, vomiting, nausea, effects on circulatory system, small decreases in heart rate, tachycardia, arrhythmias, premature ventricular contractions and vasodilation. Overdosage may cause death, emesis, convulsions, excitement, mild delirium, sensory disturbances such as ringing in the ears and flashes of light, tense and tremulous muscles, extrasystoles and quickened respiration. Continued excessive use may lead to digestive disturbances, constipation, palpitations, shortness of breath and depressed mental states. Other symptoms may include pulmonary edema, myocardial infarction, ventricular fibrillation, stomach cramps, chills, cerebral edema and hypokalemia. It may also cause rapid pulse, hallucinations, photophobia, gastroenteric distress and diuresis. Anxiety and irritability may occur. Gastric irritation, headache, fever, agitation, hyperventilation and respiratory failure may also occur. Dizziness has been reported. It may also cause irritation of the skin, eyes, mucous membranes and respiratory tract. ACUTE/CHRONIC HAZARDS: This compound is harmful by ingestion, inhalation or skin absorption. It is an irritant of the skin, eyes, mucous membranes and respiratory tract. When heated to decomposition it emits toxic fumes of carbon monoxide, carbon dioxide and nitrogen oxides. (NTP, 1992)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Emergency and supportive measures: Maintain an open airway and assist ventilation if necessary. Treat seizures and hypotension if they occur. Extreme anxiety or agitation may respond to benzodiazepines such as IV lorazepam. Hypokalemia usually resolves without treatment but in severe poisonings may need treatment as it can contribute to life-threatening arrhythmias. Monitor ECG and vital signs for at least 6 hours after ingestion.

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Use water spray, powder.

5.2 Specific hazards arising from the chemical

Flash point data for this chemical are not available; however, it is probably combustible. (NTP, 1992)

5.3 Special protective actions for fire-fighters

Use water spray, dry powder.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

6.2 Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

6.3 Methods and materials for containment and cleaning up

Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs. Well closed.Separated from food and feedstuffs. Well closed.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

Component	Caffeine			
CAS No.	58-08-2			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m^3	ppm	mg/m^3
Latvia		0,5		
	Remarks			

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	PHYSICAL DESCRIPTION: Odorless white powder or white glistening needles, usually melted together. Bitter taste. Solutions in water are neutral to litmus. Odorless. (NTP, 1992)
Colour	White, prismatic crystals
Odour	Odorless
Melting point/freezing point	234-236.5 °C(lit.)
Boiling point or initial boiling point and boiling range	178°C
Flammability	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	178°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	pH = 6.9 (1% solution)
Kinematic viscosity	no data available
Solubility	10 to 50 mg/mL at 73° F (NTP, 1992)
Partition coefficient n-octanol/water	-0.07
Vapour pressure	9.0X10-7 mm Hg at 25 deg C /Extrapolated/
Density and/or relative density	1.23
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Decomposes on burning. This produces toxic fumes including nitrogen oxides.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

Combustible.CAFFEINE may be hygroscopic. Aqueous solutions (1.12 mg/mL) are stable for three weeks at 41° F if protected from light. In normal room lighting and at room temperature, solutions are stable for 3 days. Solutions of this chemical in water, DMSO, 95% ethanol or acetone should be stable for 24 hours under normal lab conditions. REACTIVITY: This compound may react with strong oxidizing agents. It is also incompatible with iodine, silver salts and tannins. This compound is a very weak base. It is decomposed by strong

solutions of caustic alkalis. (NTP, 1992)

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

When heated to decomposition, it emits toxic fumes of /nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 192 mg/kg
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Evaluation: There is inadequate evidence for the carcinogenicity in humans of caffeine. There is inadequate evidence for the carcinogenicity in experimental animals of caffeine. Overall evaluation: Caffeine is not classifiable as to its carcinogenicity to humans (Group 3).

Reproductive toxicity

no data available

STOT-single exposure

The substance may cause effects on the central nervous system and cardiovascular system. This may result in insomnia, excitement, tachycardia and polyuria.

STOT-repeated exposure

no data available

Aspiration hazard

Evaporation at 20°C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50; Species: Pimephales promelas (Fathead minnow); Conditions: freshwater, static; Concentration: 100 mg/L for 48 hr
- Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea) age < 24 hr neonate; Conditions: freshwater, static, 21 deg C; Concentration: 3.521 mM for 24 hr; Effect: intoxication, immobilization
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC: The estimated half-life for caffeine in the Rhine River, Netherlands, was 0.8 days, which was thought to occur as a result of biological removal processes(1). Caffeine was found to be readily biodegradable when incubated with a sewage sludge inoculum(2). Using OECD 301F method, biodegradation was found to be 58% in one vessel and 84% in a second vessel(3). The structurally analogous substance theophylline (differs by only one methyl group from caffeine) is readily biodegradable by OECD 301A method with 90-100% biodegradation after 22 days and >90% at the end of the 10-days-window(3). In biodegradation studies using 3 soils from Ontario Canada and a 34-day incubation period, 14C-caffeine was rapidly mineralized to 14-CO2 in a sandy loam and loam soil, and less rapidly in a silt loam soil(4); mineralization in the sandy loam and loam soils reached about 60% in 20 days (50% in 3-10 days) with mineralization in the silt loam soil reaching about 25% in 34 days(4). A microcosm study using sediments collected upstream and downstream from wastewater treatment plants found caffeine to undergo biomineralization under aerobic conditions(5).

12.3 Bioaccumulative potential

An estimated BCF of 3 was calculated for caffeine in fish(SRC), using a log Kow of -0.07(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4 Mobility in soil

The log Koc of caffeine was experimentally determined to be 2.87 and 3.89 in a silt loam soil and in a sandy loam soil respectively(1). According to a classification scheme(2), a log Koc range of 2.87 to 3.89 (Koc range of 741 to 7762) suggests that caffeine may have low mobility in soil to being immobile in soil. Sorption tests using sand approximated a log Koc value of 1.85 (Koc of 71) using an assumed organic carbon content of 0.1% in the sand(1) which would suggest high mobility(2,SRC). Caffeine is both a weak acid and a weak base with pKa values of 14.0(3) and 0.7(4). Although partial ionization to cation and anion forms may occur, electrochemical studies have found that the neutral form of caffeine was predominant in the pH range of 5.5 to 9.0(4). Cations generally adsorb more strongly to organic carbon and clay than their neutral counterparts(5) suggesting that the cation form of caffeine may have higher Koc values than the neutral form(SRC).

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN1544 (For reference only, please check.) IMDG: UN1544 (For reference only, please check.) IATA: UN1544 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.) IMDG: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.) IATA: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.) IMDG: 6.1 (For reference only, please check.) IATA: 6.1 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: I (For reference only, please check.) IMDG: I (For reference only, please check.) IATA: I (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: No IMDG: No IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Caffeine	Caffeine	58-08-2	200-362-1
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.

Korea Existing Chemicals List (KECL)	Listed.

SECTION 16: Other information

Information on revision

Creation Date	July 15, 2019
Revision Date	August 08, 2025

Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Any questions regarding this SDS, Please send your inquiry to info@cato-chem.com

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