



# Safety Data Sheet

## Caffeine-d<sub>9</sub> (1,3,7-methyl-d<sub>9</sub>)

### Section 1. Chemical product and company identifications

**Product code:** D-5972

**Chemical formula:** C<sub>8</sub>HD<sub>9</sub>N<sub>4</sub>O<sub>2</sub>

**CAS:** 72238-85-8

**CAS (unlabelled):** 58-08-2

**Synonyms:** 1,3,7-Trimethylxanthine

**Supplier / Manufacturer:**

**C/D/N Isotopes Inc.**

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Pointe-Claire (Québec) H9R 1H1

Phone: 514-697-6254

Toll-Free (Canada & USA): 1-800-565-4696

Fax: 514-697-6148

Website: www.cdnisotopes.com

**In case of emergency:**

**TOXYSCAN HOTLINE: 1-855-780-0599**

### Section 2. Hazards identifications

**GHS (Globally Harmonized System of Classification and Labelling of Chemicals):**

**GHS Classification:** - Acute toxicity, Oral (Category 4)

**GHS Label elements:** - Pictograms:   
- Signal word: Danger

**Hazards statement:** - H302 Harmful if swallowed.

**Precautionary statement:** P264 Wash skin thoroughly after handling.  
- P270 Do not eat, drink or smoke when using this product.  
- P301 + P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell. Rinse mouth.  
- P501 Dispose of contents/ container to an approved waste disposal plant.

### Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
Caffeine-d <sub>9</sub> (1,3,7-trimethyl-d <sub>9</sub> )	72238-85-8	> 98

### Section 4. First aid measures

**Eye contact:** Flush eyes with water as a precaution.

**Skin contact:** Wash off with soap and plenty of water. Consult a physician.

**Inhalation:** If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**Ingestion:** Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

**General advice:** Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**Indication of immediate medical attention and special treatment needed, if necessary:** No data available.

**Most important symptoms and effects, both acute and delayed:** No data available.

## **Section 5. Firefighting measures**

**Flammability of the product:** Not flammable or combustible.

**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides.

**Firefighting media and instructions:** Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Special protective equipment for firefighters:** Wear self-contained breathing apparatus for firefighting if necessary.

## **Section 6. Accidental release measures**

**Personal precautions:** Use personal protective equipment. Avoid dust formation. Ensure adequate ventilation. Avoid breathing dust.

**Environmental precautions:** Do not let product enter drains. Discharge into the environment must be avoided.

**Methods for cleaning up:** Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

## **Section 7. Handling and storage**

**Handling:** Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation.

**Storage:** Store at room temperature. Adequate ventilation.

## **Section 8. Exposure Controls, Personal Protections**

**Engineering controls:** Use mechanical exhaust or laboratory fumehood to avoid exposure.

**Eyes:** Safety glasses with side-shields conforming to NIOSH (US) or EN 166 (EU).

**Respiratory:** Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US).

**Hands:** Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Skin/body:** Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

## **Section 9. Physical and chemical properties (unlabelled)**

**Molecular weight:** 194.19 g/mol

**Physical status:** Solid

**Color:** White to off-white

**Odour:** No data available

**Density:** No data available

**Melting point:** 234 - 236 °C (453 - 457 °F)

**Boiling point:** No data available

**Vapour pressure:** No data available

**Vapour density:** No data available

**Partition coefficient (octanol/water):** log Pow: -0.07

**Water solubility:** 21.6 g/l

**Lower explosion limit:** No data available.

**Upper explosion limit:** No data available.

**Auto-ignition temperature:** 540 °C (1004 °F)

**Flash point:** No data available.

## **Section 10. Stability and reactivity**

**Stability and reactivity:** Stable under recommended storage conditions.

**Incompatibility:** Strong oxidizing agents.

**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides.

**Reactivity conditions:** No data available

## **Section 11. Toxicological information (unlabelled)**

**Toxicological data:** Caffeine

### **Information on ingredients:**

<b><u>Name</u></b>	<b><u>CAS</u></b>	<b><u>LD<sub>50</sub></u></b>	<b><u>LC<sub>50</sub></u></b>
Caffeine	58-08-2	Oral - Rat - 192 mg/kg Dermal - Rat > 2000 mg/kg	No data available

### **Potential acute effects**

- **Eyes:** No data available.
- **Skin:** No data available.
- **Inhalation:** No data available.
- **Ingestion:** Harmful if swallowed.

### **Potential chronic effects**

- **Carcinogenic effects:** IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Caffeine). ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** Genotoxicity in vitro - rat - Kidney. Micronucleus test. Genotoxicity in vivo - mouse - Oral. Micronucleus test.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

## **Section 12. Ecological information**

### **Ecological data:**

<b><u>Name</u></b>	<b><u>Results</u></b>	<b><u>Species</u></b>	<b><u>Period</u></b>
Caffeine	87 mg/l LC50 182 mg/l EC50	Leuciscus idus Daphnia magna	96 h 48 h

**Effects on environment:** An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

**Mobility:** No data available

**Environmental precautions:** No data available

**Persistence and degradability:** No data available

**Bioaccumulative potential:** No data available

## **Section 13. Disposal considerations**

**Waste disposal:** Contact a licensed professional waste disposal service to dispose of this material.

## **Section 14. Transportation information**

### **Classification DOT/IMDG/IATA label:**

**Shipping name:** Not dangerous goods

**UN number:** None

**Class:** None

**Packaging group:** None

**Additional information:** None

## **Section 15. Regulatory information**

### **UNITED STATES: NFPA classification**



Health: 2  
Flammable: 0  
Reactivity: 0  
Special conditions: None

**Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous**

### **U.S. Federal regulations:**

**California proposition 65 requirements** : Not Listed  
**SARA section 313 (specific toxic chemical listings)** : Not listed  
**CERCLA reportable quantity** : Not listed  
**Sections 302-304 reportable quantity** : Not listed  
**Community Right-to-Know (Sections 311 and 312)** : Not Listed

## **Section 16. Additional information**

**Date of issue:** February 7<sup>th</sup>, 2024

**Version:** 4

**Elaborated by:** Toxyscan Inc., 1-866-780-0599

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*This safety data sheet has been prepared in accordance with the OSHA (USA), WHMIS (Canada) / GHS classification rules in effect at the time of writing.*