Safety Data Sheet

Caffeine-d_3 (1-methyl-d_3)

Section 1. Chemical product and company identifications

Product code: D-5912
Chemical formula: $C_8H_7D_3N_4O_2$
CAS: 26351-03-1
CAS (unlabelled): 58-08-2
Synonyms: 1,3,7-Trimethylxanthine

Supplier / Manufacturer:

C/D/N Isotopes Inc.
88 Leacock Street
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

Name	CAS	Concentration %
Caffeine-d_3 (1-methyl-d_3)	26351-03-1	> 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.

©2015 All rights reserved C/D/N Isotopes, Inc. / Toxyscan, Inc.

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

©2015 All rights reserved C/D/N Isotopes, Inc. / Toxyscan, Inc.

Section 11. Toxicological information (unlabelled)

Toxicological data: Caffeine

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
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:

Name	Results	Species	Period
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

©2015 All rights reserved C/D/N Isotopes, Inc. / Toxyscan, Inc.

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 7th, 2024**
Version: 4
Elaborated by: **Toxyscan Inc., 1-866-780-0599**
Notice to reader: To the best of our knowledge, the information contained herein is accurate. However, C/D/N Isotopes Inc., Toxyscan Inc., or 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 materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

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.

©2015 All rights reserved C/D/N Isotopes, Inc. / Toxyscan, Inc.