



# CAFFEINE (TRIMETHYL-13C3, 99%)

## Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

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CLM-514

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1. Product identifier

Product form	: Substance
Substance name	: CAFFEINE (TRIMETHYL-13C3, 99%)
EC Index-No.	: 613-086-00-5 (Unlabeled)
EC-No.	: 200-362-1 (Unlabeled)
CAS-No.	: 78072-66-9
Product code	: CLM-514
Formula	: *C3C5H10N4O2
Synonyms	: 1,3,7-Trimethylxanthine

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

#### 1.2.1. Relevant identified uses

Main use category	: Professional use
Industrial/Professional use spec	: For professional use only

#### 1.2.2. Uses advised against

No additional information available

### 1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.  
50 Frontage Road  
Andover, MA 01810  
USA

USA: 1-800-322-1174 Int: 1-978-749-8000

[cilsales@isotope.com](mailto:cilsales@isotope.com) [www.isotope.com](http://www.isotope.com)

### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)

International: 1-703-741-5970 (24 hours)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

#### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute Tox. 4 (Oral) H302

Full text of hazard classes and H-statements : see section 16

#### Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

Xn; R22

Full text of R-phrases: see section 16

#### GHS-US classification

Acute Tox. 4 (Oral) H302

Full text of H statements : see section 16

#### Adverse physicochemical, human health and environmental effects

No additional information available

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### 2.2. Label elements

#### Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H302 - Harmful if swallowed.

Precautionary statements (CLP) :

P264 - Wash hands, forearms and face thoroughly after handling.  
P270 - Do not eat, drink or smoke when using this product.  
P301+P312 - IF SWALLOWED: Call a doctor if you feel unwell.  
P330 - Rinse mouth.  
P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

#### GHS-US labelling

Hazard pictograms (GHS-US) :



GHS07

Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

H302 - Harmful if swallowed.

Precautionary statements (GHS-US) :

P264 - Wash hands, forearms and face thoroughly after handling.  
P270 - Do not eat, drink or smoke when using this product.  
P301+P312 - If swallowed: Call a doctor if you feel unwell  
P330 - Rinse mouth.  
P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

Name	Product identifier	%	Classification according to Directive 67/548/EEC
CAFFEINE (TRIMETHYL-13C3, 99%)	(CAS-No.) 78072-66-9 (EC-No.) 200-362-1 (Unlabeled) (EC Index-No.) 613-086-00-5 (Unlabeled)	100	Xn; R22

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
CAFFEINE (TRIMETHYL-13C3, 99%)	(CAS-No.) 78072-66-9 (EC-No.) 200-362-1 (Unlabeled) (EC Index-No.) 613-086-00-5 (Unlabeled)	100	Acute Tox. 4 (Oral), H302

Full text of R- and H-statements: see section 16

Name	Product identifier	%	GHS-US classification
CAFFEINE (TRIMETHYL-13C3, 99%) (Main constituent)	(CAS-No.) 78072-66-9	100	Acute Tox. 4 (Oral), H302

Full text of H-statements: see section 16

### 3.2. Mixtures

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general : If you feel unwell, seek medical advice (show the label where possible). Evacuate danger area.

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First-aid measures after inhalation	: When symptoms occur: go into open air and ventilate suspected area. If not breathing, give artificial respiration. Get medical advice/attention.
First-aid measures after skin contact	: Wash with plenty of water/.... Get immediate medical advice/attention.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention. Call a POISON CENTER/doctor if you feel unwell.

### 4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory irritation.
Symptoms/effects after skin contact	: May be harmful in contact with skin. May cause moderate irritation.
Symptoms/effects after eye contact	: May cause eye irritation.
Symptoms/effects after ingestion	: Harmful if swallowed. Swallowing a small quantity of this material will result in serious health hazard.

### 4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : Water spray. Dry chemical powder, alcohol-resistant foam, carbon dioxide (CO2).

### 5.2. Special hazards arising from the substance or mixture

No additional information available

### 5.3. Advice for firefighters

Firefighting instructions	: Fight fire with normal precautions from a reasonable distance. Wear a self contained breathing apparatus. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection. Wear recommended personal protective equipment.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

#### 6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment as required. Avoid breathing vapours, mist, gas. Avoid dust formation. Ensure adequate ventilation.

#### 6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

### 6.2. Environmental precautions

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

### 6.3. Methods and material for containment and cleaning up

For containment	: Take up mechanically (sweeping, shovelling) and collect in suitable container for disposal.
Methods for cleaning up	: This material and its container must be disposed of in a safe way, and as per local legislation.

### 6.4. Reference to other sections

For further information refer to section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Precautions for safe handling	: Provide adequate ventilation to minimize dust and/or vapour concentrations. Avoid contact with eyes. Avoid contact with skin. Avoid breathing dust, mist or spray.
Hygiene measures	: Handle in accordance with good industrial hygiene and safety practice. Do not eat, drink or smoke when using this product. Wash hands, forearms and face thoroughly after handling.

### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures	: Store in a well-ventilated place. Keep container tightly closed.
Storage conditions	: Store at room temperature away from light and moisture.

### 7.3. Specific end use(s)

No additional information available

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No additional information available

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### 8.2. Exposure controls

- Appropriate engineering controls : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.
- Personal protective equipment : Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.



- Materials for protective clothing : Wear suitable protective clothing and gloves.
- Hand protection : Wear suitable protective clothing and gloves.
- Eye protection : Wear eye protection. Chemical goggles or face shield with safety glasses.
- Skin and body protection : Wear suitable protective clothing, gloves and eye/face protection.
- Respiratory protection : In case of inadequate ventilation wear respiratory protection. Approved supplied air respirator.
- Environmental exposure controls : Avoid release to the environment.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

- Physical state : Solid
- Appearance : Powder
- Molecular mass : 197.17 g/mol (Labeled)
- Colour : White
- Odour : No data available
- Odour threshold : No data available
- pH : 5.5 - 6.5 at 10 g/l at 20 °C (68 °F)
- Relative evaporation rate (butylacetate=1) : No data available
- Melting point : 234 - 236 °C (453 - 457.7 °F) - lit.
- Freezing point : No data available
- Boiling point : No data available
- Flash point : No data available
- Auto-ignition temperature : No data available
- Decomposition temperature : No data available
- Flammability (solid, gas) : No data available
- Vapour pressure : 20 hPa (15 mmHg) at 89 °C (192 °F)
- Relative vapour density at 20 °C : No data available
- Relative density : 1.23 g/cm<sup>3</sup> at 18 °C (64 °F)
- Solubility : Water: 18.7 g/l at 16 °C (61 °F)
- Log Pow : -0.091 at 23 °C (73 °F)
- Log Kow : No data available
- Viscosity, kinematic : No data available
- Viscosity, dynamic : No data available
- Explosive properties : No data available
- Oxidising properties : No data available
- Explosive limits : No data available

### 9.2. Other information

- Additional information : Bulk density 220 kg/m<sup>3</sup>. Dissociation constant 10.4 at 40 °C (104 °F)

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

No additional information available

### 10.2. Chemical stability

Stable if stored under recommended conditions.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

No additional information available

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### 10.5. Incompatible materials

Strong oxidizing agents.

### 10.6. Hazardous decomposition products

No additional information available

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed.

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
LD50 oral rat	367.7 mg/kg - male and female (OECD Test Guideline 401)
LD50 dermal	> 2000 mg/kg - male and female
LC50 inhalation rat (mg/l)	4.94 mg/l - male and female (Calculation method)
ATE CLP (oral)	500.000 mg/kg bodyweight

Skin corrosion/irritation : Skin - Rabbit Result: No skin irritation. (OECD Test Guideline 404)  
pH: 5.5 - 6.5 at 10 g/l at 20 °C (68 °F)

Serious eye damage/irritation : Eyes. rabbit. Result: No eye irritation. (OECD Test Guideline 405)  
pH: 5.5 - 6.5 at 10 g/l at 20 °C (68 °F)

Respiratory or skin sensitisation : Not classified

Germ cell mutagenicity : rat Kidney Micronucleus test mouse Micronucleus test

Carcinogenicity : Not classified

Reproductive toxicity : Not classified

STOT-single exposure : Not classified

STOT-repeated exposure : Not classified

Aspiration hazard : Not classified

Potential adverse human health effects and symptoms : This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product. Harmful if swallowed. Liver - Irregularities - Based on Human Evidence.

IARC group : 3

Symptoms/effects after inhalation : May be harmful if inhaled. May cause respiratory irritation.

Symptoms/effects after skin contact : May be harmful in contact with skin. May cause moderate irritation.

Symptoms/effects after eye contact : May cause eye irritation.

Symptoms/effects after ingestion : Harmful if swallowed. Swallowing a small quantity of this material will result in serious health hazard.

## SECTION 12: Ecological information

### 12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms nor to cause long-term adverse effects in the environment.

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
LC50 fish 1	87 mg/l - Leuciscus idus (Golden orfe) - 96 h
EC50 Daphnia 1	182 mg/l static test - Daphnia magna (Water flea) - 48 h (DIN 38412)
ErC50 (algae)	Toxicity to algae static test - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)

### 12.2. Persistence and degradability

No additional information available

### 12.3. Bioaccumulative potential

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
Log Pow	-0.091 at 23 °C (73 °F)

### 12.4. Mobility in soil

No additional information available

### 12.5. Results of PBT and vPvB assessment

No additional information available

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### 12.6. Other adverse effects

No additional information available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

- Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.
- Product/Packaging disposal recommendations: : Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
- Ecology - waste materials : Dispose of as unused product.

## SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

### 14.1. UN number

Not applicable

### 14.2. UN proper shipping name

Not applicable

### 14.3. Additional information

- Other information : No supplementary information available.
- Special transport precautions : Not dangerous.

#### Overland transport

No additional information available

#### Transport by sea

No additional information available

#### Air transport

No additional information available

### 14.4. Environmental hazards

- Other information : No supplementary information available.

### 14.5. Special precautions for user

- Special transport precautions : Not dangerous.

### 14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Delayed (chronic) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313.

### 15.2. International regulations

#### CANADA

CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)
Listed on the Canadian DSL (Domestic Substances List)

#### 15.2.1. National regulations

No additional information available

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### 15.3. US State regulations

CAFFEINE (TRIMETHYL-13C3, 99%)(78072-66-9)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	RTK - U.S. - Pennsylvania - RTK (Right to Know) List RTK - U.S. - New Jersey - Right to Know Hazardous Substance List

### SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

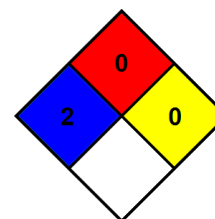
Full text of R-, H- and EUH-statements:

Acute Tox. 4 (Oral)	Acute toxicity (oral), Category 4
H302	Harmful if swallowed.
R22	Harmful if swallowed
Xn	Harmful

NFPA health hazard : 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard : 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



### HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 0 Minimal Hazard

Physical : 0 Minimal Hazard

CIL Substance SDS

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