

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 2015/830 and US OSHA HCS 2015

**Section 1. Identification of the Substance/Mixture and of the Company/Undertaking**

- 1.1 Product Code:** 27972  
**Product Name:** Caffeine-13C3 (CRM)  
**Synonyms:** 3,7-dihydro-1,3,7-tri(methyl-13C)-1H-purine-2,6-dione; Methyltheobromine-13C3;
- 1.2 Relevant identified uses of the substance or mixture and uses advised against:**  
**Relevant identified uses:** For research use only, not for human or veterinary use.
- 1.3 Details of the Supplier of the Safety Data Sheet:**  
**Company Name:** Cayman Chemical Company  
 1180 E. Ellsworth Rd.  
 Ann Arbor, MI 48108  
**Web site address:** www.caymanchem.com  
**Information:** Cayman Chemical Company +1 (734)971-3335
- 1.4 Emergency telephone number:**  
**Emergency Contact:** CHEMTREC Within USA and Canada: +1 (800)424-9300  
 CHEMTREC Outside USA and Canada: +1 (703)527-3887

**Section 2. Hazards Identification**

- 2.1 Classification of the Substance or Mixture:**  
**Flammable Liquids, Category 2**  
**Acute Toxicity: Inhalation, Category 3**  
**Acute Toxicity: Oral, Category 3**  
**Acute Toxicity: Skin, Category 3**  
**Specific Target Organ Toxicity (single exposure), Category 1**

**2.2 Label Elements:**



**GHS Signal Word:** **Danger**

**GHS Hazard Phrases:**

- H225: Highly flammable liquid and vapor.  
 H301: Toxic if swallowed.  
 H311: Toxic in contact with skin.  
 H331: Toxic if inhaled.  
 H370: Causes damage to organs.

**GHS Precautionary Phrases:**

- P210: Keep away from {heat/sparks/open flames/hot surfaces}. - No smoking.  
 P260: Do not breathe {dust/fume/gas/mist/vapors/spray}.  
 P264: Wash {hands} thoroughly after handling.  
 P280: Wear {protective gloves/protective clothing/eye protection/face protection}.

**GHS Response Phrases:**

- P301+310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.  
 P302+352: IF ON SKIN: Wash with plenty of soap and water.  
 P303+361+353: IF ON SKIN (or hair): Remove/take off immediately all contaminated clothing. Rinse skin with water/shower.  
 P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.  
 P307+311: IF exposed: Call a POISON CENTER or doctor/physician.

P311: Call a POISON CENTER or doctor/physician.  
 P330: Rinse mouth.  
 P361: Remove/Take off immediately all contaminated clothing.  
 P363: Wash contaminated clothing before reuse.

**GHS Storage and Disposal Phrases:**

Please refer to Section 7 for Storage and Section 13 for Disposal information.

**2.3 Adverse Human Health** Causes damage to organs {eyes}.

**Effects and Symptoms:** Material may be irritating to the mucous membranes and upper respiratory tract.  
 May be fatal or cause blindness if swallowed.  
 May cause eye, skin, or respiratory system irritation.  
 Toxic if inhaled, swallowed, or in contact with skin.  
 To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

**Section 3. Composition/Information on Ingredients**

CAS # / RTECS #	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	GHS Classification
78072-66-9 NA	Caffeine-13C3	0.1 %	693-114-0 NA	Acute Tox.(O) 4: H302
67-56-1 PC1400000	Methanol 01-2119392409-28-0000	99.9 %	200-659-6 603-001-00-X	Flam. Liq. 2: H225 Acute Tox.(O) 3: H301 Acute Tox.(D) 3: H311 Acute Tox.(I) 3: H331 STOT (SE) 1: H370

**Section 4. First Aid Measures**

**4.1 Description of First Aid Measures:**

**In Case of Inhalation:** Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.

**In Case of Skin Contact:** Immediately wash skin with soap and plenty of water for at least 15 minutes. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

**In Case of Eye Contact:** Hold eyelids apart and flush eyes with plenty of water for at least 15 minutes. Have eyes examined and tested by medical personnel.

**In Case of Ingestion:** Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.

**4.2 Important Symptoms and Effects, Both Acute and Delayed:** Overexposure may cause: confusion, dermatitis, headache, drowsiness, dizziness, gastrointestinal disturbance, optic nerve damage (blindness), nausea, unconsciousness, vomiting, visual disturbance, weakness.  
 May cause convulsions.  
 Once methanol is absorbed into the body, it is very slowly eliminated.

### Section 5. Fire Fighting Measures

- 5.1 Suitable Extinguishing** Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.  
**Media:** Use water spray to cool fire-exposed containers.  
**Unsuitable Extinguishing** A solid water stream may be inefficient.  
**Media:**
- 5.2 Flammable Properties and Hazards:** Can release vapors that form explosive mixtures at temperatures at or above the flashpoint.  
 Container explosion may occur under fire conditions.  
 Emits toxic fumes under fire conditions.  
 Sensitive to static discharge.  
 Vapors can travel to a source of ignition and flash back.  
 No data available.  
**Flash Pt:** 11.00 C Method Used: Closed Cup  
**Explosive Limits:** LEL: 6.0% at 25.0 C UEL: 36.0% at 25.0 C  
**Autoignition Pt:** 385.00 C
- 5.3 Fire Fighting Instructions:** As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.  
 Note: Flammable as diluted in methanol.

### Section 6. Accidental Release Measures

- 6.1 Protective Precautions,** Avoid breathing vapors and provide adequate ventilation.  
**Protective Equipment and Emergency Procedures:** As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator, and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
- 6.2 Environmental Precautions:** Take steps to avoid release into the environment, if safe to do so.
- 6.3 Methods and Material For Containment and Cleaning Up:** Contain spill and collect, as appropriate.  
 Transfer to a chemical waste container for disposal in accordance with local regulations.

### Section 7. Handling and Storage

- 7.1 Precautions To Be Taken in Handling:** Avoid breathing dust/fume/gas/mist/vapours/spray.  
 Avoid prolonged or repeated exposure.  
 Keep away from sources of ignition.  
 Take precautionary measures against static discharge.
- 7.2 Precautions To Be Taken in Storing:** Keep away from heat, sparks, and flame.  
 Keep container tightly closed.  
 Store in accordance with information listed on the product insert.

### Section 8. Exposure Controls/Personal Protection

**8.1 Exposure Parameters:**

CAS #	Chemical Name	Jurisdiction	Recommended Exposure Limits	Notations
67-56-1	Methanol	ACGIH TLV	TLV: 200 ppm STEL: 250 ppm	
		Europe	TWA: 260 mg/m3 (200 ppm)	Skin Absorption
		France VL	TWA: 260 mg/m3 (200 ppm) STEL: 1300 mg/m3 (1000 ppm)	
		OSHA PELs	PEL: 200 ppm	
		Britain EH40	TWA: 266 mg/m3 (200 ppm) STEL: 333 mg/m3 (250 ppm)	Skin Absorption

**8.2 Exposure Controls:**

**8.2.1 Engineering Controls (Ventilation etc.):** Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.

**8.2.2 Personal protection equipment:**

**Eye Protection:** Safety glasses

**Protective Gloves:** Compatible chemical-resistant gloves

**Other Protective Clothing:** Lab coat

**Respiratory Equipment (Specify Type):** NIOSH approved respirator, as conditions warrant.

**Work/Hygienic/Maintenance Practices:** Do not take internally.

Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower. Wash thoroughly after handling.

No data available.

**Section 9. Physical and Chemical Properties**

**9.1 Information on Basic Physical and Chemical Properties**

**Physical States:** [ ] Gas [X] Liquid [ ] Solid

**Appearance and Odor:** A 1 mg/ml solution in methanol

**pH:** No data.

**Melting Point:** No data.

**Boiling Point:** No data.

**Flash Pt:** 11.00 C Method Used: Closed Cup

**Evaporation Rate:** No data.

**Flammability (solid, gas):** No data available.

**Explosive Limits:** LEL: 6.0% at 25.0 C UEL: 36.0% at 25.0 C

**Vapor Pressure (vs. Air or mm Hg):** 96 MM\_HG at 20.0 C

**Vapor Density (vs. Air = 1):** No data.

**Specific Gravity (Water = 1):** No data.

**Solubility in Water:** No data.

**Octanol/Water Partition Coefficient:** No data.

**Autoignition Pt:** 385.00 C

**Decomposition Temperature:** No data.

**Viscosity:** No data.

**9.2 Other Information**

**Percent Volatile:** No data.

**Molecular Formula & Weight:** C<sub>5</sub>[<sup>13</sup>C]<sub>3</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub> 197.2

### Section 10. Stability and Reactivity

<b>10.1 Reactivity:</b>	No data available.
<b>10.2 Stability:</b>	Unstable [ ]    Stable [ X ]
<b>10.3 Stability Note(s):</b>	Stable if stored in accordance with information listed on the product insert.
<b>Polymerization:</b>	Will occur [ ]    Will not occur [ X ]
<b>10.4 Conditions To Avoid:</b>	heat, flames, and sparks
<b>10.5 Incompatibility - Materials To Avoid:</b>	acids acid anhydrides acid chlorides alkali metals oxidizing agents reducing agents
<b>10.6 Hazardous Decomposition or Byproducts:</b>	carbon dioxide carbon monoxide

### Section 11. Toxicological Information

<b>11.1 Information on Toxicological Effects:</b>	The toxicological effects of this product have not been thoroughly studied. Methanol - Toxicity Data: Oral LD50 (rat): 5,600 mg/kg; Oral LD50 (rabbit): 14,200 mg/kg; Oral LDLO (man): 6422 mg/kg; Intraperitoneal LD50 (mouse): 10765 mg/kg; Inhalation LC50 (rat): 64,000 ppm (4h); Inhalation LC50 (mouse): 61,100 ppm (134 m); Skin LD50 (rabbit): 15,800 mg/kg; Oral LDLO (human): 143 mg/kg; Methanol - Irritation Data: Skin (rabbit): 20 mg (24h) moderate; Eyes (rabbit): 40 mg moderate; Eyes (rabbit): 100 mg (24h) moderate;
<b>Chronic Toxicological Effects:</b>	Methanol - Investigated as a drug, mutagen, primary irritant, reproductive effector, and tumorigen. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information. Methanol RTECS Number: PC1400000
<b>Carcinogenicity:</b>	NTP? No    IARC Monographs? No    OSHA Regulated? No

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
78072-66-9	Caffeine-13C3	n.a.	n.a.	n.a.	n.a.
67-56-1	Methanol	n.a.	n.a.	n.a.	n.a.

### Section 12. Ecological Information

<b>12.1 Toxicity:</b>	Avoid release into the environment. Runoff from fire control or dilution water may cause pollution.
<b>12.2 Persistence and Degradability:</b>	No data available.
<b>12.3 Bioaccumulative Potential:</b>	No data available.
<b>12.4 Mobility in Soil:</b>	No data available.
<b>12.5 Results of PBT and vPvB assessment:</b>	No data available.
<b>12.6 Other adverse effects:</b>	No data available.

**Section 13. Disposal Considerations**

**13.1 Waste Disposal Method:** Dispose in accordance with local, state, and federal regulations.

**Section 14. Transport Information**

**14.1 LAND TRANSPORT (US DOT):**

**DOT Proper Shipping Name:** Methanol Solution  
**DOT Hazard Class:** 3 (6.1) FLAMMABLE LIQUID, POISON  
**UN/NA Number:** UN1230 **Packing Group:** II



**14.1 LAND TRANSPORT (European ADR/RID):**

**ADR/RID Shipping Name:** Methanol Solution  
**UN Number:** 1230 **Packing Group:** II  
**Hazard Class:** 3 (6.1) - FLAMMABLE LIQUID, POISON

**14.3 AIR TRANSPORT (ICAO/IATA):**

**ICAO/IATA Shipping Name:** Methanol Solution  
**UN Number:** 1230 **Packing Group:** II  
**Hazard Class:** 3 (6.1) - FLAMMABLE LIQUID, POISON **IATA Classification:** 3, 6.1

**Additional Transport Information:** Transport in accordance with local, state, and federal regulations.  
 When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10.  
 Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

**Section 15. Regulatory Information**

**EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists**

CAS #	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
78072-66-9	Caffeine-13C3	No	No	No
67-56-1	Methanol	No	Yes 5000 LB	Yes

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
78072-66-9	Caffeine-13C3	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No
67-56-1	Methanol	CAA HAP,ODC: HAP: VHAP; CWA NPDES: No; TSCA: Yes - Inventory; CA PROP.65: Yes: RDTox.

<b>Regulatory Information Statement:</b>	This SDS was prepared in accordance with 29 CFR 1910.1200 and Regulation (EC) No.1272/2008.
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## Section 16. Other Information

<b>Revision Date:</b>	09/19/2019
<b>Additional Information About This Product:</b>	No data available.
<b>Company Policy or Disclaimer:</b>	DISCLAIMER: This information is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.