



# Safety Data Sheet - Version 5.0

Preparation Date 9/21/2015

Latest Revision Date (If Revised)

SDS Expiry Date 9/19/2018

## 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1 Product Identifier

**Chemical Name** 1-(3-Carboxypropyl)-3,7-dimethylxanthine

**Catalogue #** C181235

### 1.2 Relevant Identified Uses of the Substance or Mixture and Uses Advised Against

**Product Uses** To be used only for scientific research and development. Not for use in humans or animals.

### 1.3 Details of the Supplier of the Safety Data Sheet

**Company** Toronto Research Chemicals  
2 Brisbane Road  
Toronto, ON M3J 2J8  
CANADA

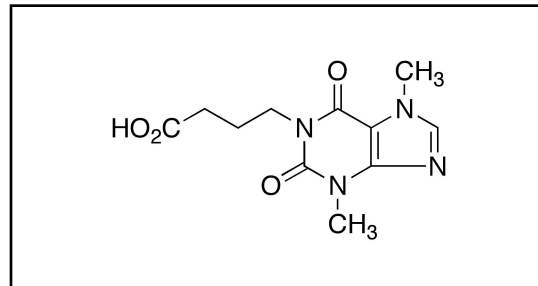
**Telephone** +14166659696

**FAX** +14166654439

**Email** orders@trc-canada.com

### 1.4 Emergency Telephone Number

**Emergency#** +14166659696 between 0800-1700 (GMT-5)



## 2. HAZARDS IDENTIFICATION

### WHMIS Classification (Canada)

None Not WHMIS controlled.

### WHMIS Symbols (Canada)

### 2.1/2.2 Classification of the Substance or Mixture and Label Elements

#### GHS Hazards Classification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

Not a hazardous substance by GHS.

#### EU Classification (According to EU Regulation 67/548/EEC)

Not a hazardous substance by this Classification.

#### EU Risk and Safety Statements (According to EU Regulation 67/548/EEC)

**Hazard Statements** **Hazard Codes**

None

#### Risk Codes and Phrases

None Not a hazardous substance by this Classification.

#### Safety Precaution Codes and Phrases

#### GHS Hazards Identification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

**Signal Word** None

#### GHS Hazard Statements

None Not a hazardous substance according to GHS.

## GHS Precautionary Statements

### 2.3 Unclassified Hazards/Hazards Not Otherwise Classified

No data available.

## **3. COMPOSITION/INFORMATION ON INGREDIENTS**

### 3.1 Substances

**Molecular Formula:** C<sub>11</sub>H<sub>14</sub>N<sub>4</sub>O<sub>4</sub>

**Molecular Weight:** 266.25

**CAS Registry #:** 6493-07-8

**EC#:**

#### **Synonyms**

2,3,6,7-Tetrahydro-3,7-dimethyl-2,6-dioxo-1H-purine-1-butanoic Acid; 3,6-Dihydro-3,7-dimethyl-2,6-dioxopurine-1 (2H)-butyric Acid; 1-(3-Carboxypropyl)theobromine; 1-(3'-Carboxypropyl)-3,7-dimethylxanthine; 3,7-Dimethyl-1-(3-carboxypropyl)xanthine;

### 3.2 Mixtures

Not a mixture.

## **4. FIRST AID MEASURES**

### 4.1 Description of First Aid Measures

#### **General Advice**

If medical attention is required, show this safety data sheet to the doctor.

#### **If Inhaled**

If inhaled, move person to fresh air. If not breathing, give artificial respiration and consult a physician.

#### **In Case of Skin Contact**

Wash affected area with soap and water. Consult a physician if any exposure symptoms are observed.

#### **In Case of Eye Contact**

Immediately rinse eyes with plenty of water for at least 15 minutes. Consult a physician.

#### **If Swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water. Do NOT induce vomiting unless advised to do so by a physician or Poison Control Center. Seek medical attention.

### 4.2 Most Important Symptoms and Effects, Both Acute and Delayed

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or in section 11.

### 4.3 Indication of any Immediate Medical Attention and Special Treatment Needed

No data available.

## **5. FIREFIGHTING MEASURES**

### 5.1 Extinguishing Media

#### **Conditions of flammability**

Not flammable or combustible.

#### **Suitable extinguishing media**

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.

### 5.2 Special Hazards Arising from the Substance or Mixture

Carbon oxides, Nitrogen oxides

### 5.3 Advice for Firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

#### **5.4 Further Information**

No data available.

### **6. ACCIDENTAL RELEASE MEASURES**

#### **Personal precautions**

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

#### **Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

#### **Method and materials for containment and cleaning up**

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### **7. HANDLING AND STORAGE**

#### **Precautions for safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed.

#### **Conditions for safe storage**

Keep container tightly closed in a dry and well-ventilated place.  
Keep in a dry place.

Storage conditions: -20°C Freezer

#### **7.3 Specific End Uses**

For scientific research and development only. Not for use in humans or animals.

### **8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

#### **8.1 Control Parameters**

Contains no components with established occupational exposure limits.

#### **8.2 Exposure Controls**

##### **Appropriate Engineering Controls**

A laboratory fumehood or other appropriate form of local exhaust ventilation should be used to avoid exposure.

##### **Personal Protective Equipment**

All recommendations below are advisory in nature and a risk assessment should be performed by the employer/end user prior to use of this product. The type of protective equipment must be selected based on the amount and concentration of the dangerous material being used in the workplace.

##### **Eye/Face Protection**

Safety goggles or face shield. All equipment should have been tested and approved under appropriate standards, such as NIOSH (US), CSA (Canada), or EN 166 (EU).

##### **Skin Protection**

Gloves should be used when handling this material. Gloves are to be inspected prior to use. Contaminated gloves are to be removed using proper glove removal technique so that the outer surface of the glove does not contact bare skin. Dispose of contaminated gloves after use in compliance with good laboratory practices and local requirements.

Gloves used for incidental exposures (splash protection) should be designated as "chemical resistant" by EU standard EN 374 with the resistance codes corresponding to the anticipated use of the material. Unrated gloves are not recommended.

Suggested gloves: AnsellPro Sol-Vex nitrile gloves style 37-175, 15 mil thickness.  
Penetration time has not been determined.

Gloves used for prolonged direct exposure (immersion) should be designated "chemical resistant" as per EN 734 with the resistance codes corresponding to the anticipated use of the material.

Suggested gloves: AnsellPro Viton/Butyl gloves style 38-612, 4/8 mil thickness.  
Penetration time has not been determined.

These recommendations may not apply if the material is mixed with any other chemical, or dissolved into a solution. A risk assessment must be performed to ensure the gloves will still offer acceptable protection.

## Body Protection

Fire resistant (Nomex) coveralls or chemical-resistant bodysuit (laminated Tychem SL or equivalent).

## Respiratory Protection

Recommended respirators are NIOSH-approved N100 or CEN-approved FFP3 particulate respirators. These are to be only used as a backup to local exhaust ventilation or other engineering controls. If the respirator is the only means of protection, a full-face supplied air respirator must be used.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on Basic Physical and Chemical Properties

#### A) Appearance

White to Off-White Solid

#### C) Odour Threshold

No data available.

#### E) Melting Point/Freezing Point

208-210°C

#### G) Flash point

No data available.

#### I) Flammability (Solid/Gas)

No data available.

#### K) Vapour Pressure

No data available.

#### M) Relative Density

No data available.

#### O) Partition Coefficient: n-octanol/water

No data available.

#### Q) Decomposition Temperature

No data available.

#### S) Explosive Properties

No data available.

#### B) Odour

No data available.

#### D) pH

No data available.

#### F) Initial Boiling Point/Boiling Range

No data available.

#### H) Evaporation Rate

No data available.

#### J) Upper/Lower Flammability/Explosive Limits

No data available.

#### L) Vapour Density

No data available.

#### N) Solubility

DMSO, Methanol

#### P) Auto-Ignition Temperature

No data available.

#### R) Viscosity

No data available.

#### T) Oxidizing Properties

No data available.

### 9.2 Other Information

no data available

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available.

### 10.2 Chemical Stability

Stable under recommend storage conditions.

### 10.3 Possibility of Hazardous Reactions

No data available.

### 10.4 Conditions to Avoid

No data available.

### 10.5 Incompatible Materials

Strong oxidizing agents.

### 10.6 Hazardous Decomposition Products

In the event of fire: See section 5. Other decomposition products: No data available.

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on Toxicological Effects

#### A) Acute Toxicity

Oral LD50: No data available.

Inhalation LC50: No data available.

Dermal LD50: No data available.

#### B) Skin Corrosion/Irritation

No data available

#### C) Serious Eye Damage/Irritation

No data available

**D) Respiratory or Skin Sensitization**

No data available

**E) Germ Cell Mutagenicity**

No data available

**F) Carcinogenicity**

No data available

**G) Reproductive Toxicity/Teratogenicity**

No data available

**H) Single Target Organ Toxicity - Single Exposure**

No data available

**I) Single Target Organ Toxicity - Repeated Exposure**

No data available

**J) Aspiration Hazard**

No data available

**K) Potential Health Effects and Routes of Exposure**

**Inhalation**

May be harmful if inhaled. May cause respiratory tract irritation.

**Ingestion**

May be harmful if swallowed.

**Skin**

May be harmful if absorbed through skin. May cause skin irritation.

**Eyes**

May cause eye irritation.

**L) Signs and Symptoms of Exposure**

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or in section 11.

To the best of our knowledge, the chemical, physical, and toxicological properties of this material have not been thoroughly investigated.

**M) Additional Information**

RTECS: Not available.

**12. ECOLOGICAL INFORMATION**

**12.1 Toxicity**

No data available.

**12.2 Persistence and Degradability**

No data available.

**12.3 Bioaccumulative Potential**

No data available.

**12.4 Mobility in Soil**

No data available.

**12.5 Results of PBT and vPvB Assessment**

No data available.

**12.6 Other Adverse Effects**

No data available.

**13. DISPOSAL CONSIDERATIONS**

**13.1 Waste Treatment Methods**

**A) Product**

Product may be burned in an incinerator equipped with afterburner and scrubber. Excess and expired materials are to be offered to a licensed hazardous material disposal company. Ensure that all Federal and Local regulations regarding the disposal and destruction of this material are followed.

**B) Contaminated Packaging**

Dispose of as above.

**C) Other Considerations**

Product is not to be disposed of in sanitary sewers, storm sewers, or landfills.

**14. TRANSPORT INFORMATION**

**14.1 UN Number**

DOT (US): N/A IATA: N/A IMDG: N/A ADR/RID: N/A

**14.2 UN Proper Shipping Name**DOT (US)/IATA:  
Not dangerous goods.  
IMDG/ARD/RID:  
Not dangerous goods.**14.3 Transport Hazard Class(es)**

DOT (US): N/A IATA: N/A IMDG: N/A ADR/RID: N/A

**14.4 Packing Group**

DOT (US): N/A IATA: N/A IMDG: N/A ADR/RID: N/A

**14.5 Environmental Hazards**

DOT (US): None IATA: None IMDG: None ADR/RID: None

**14.6 Special Precautions for User**

None

**15. REGULATORY INFORMATION**

This safety data sheet complies with the requirements of WHMIS (Canada), OSHA 1910.1200 (US), and EU Regulation EC No. 1907/2006 (European Union).

**15.1 Safety, Health and Environmental Regulations/Legislation Specific for the Substance or Mixture****A) Canada****DSL/NDSL Status:** This product is not listed on the Canadian DSL/NDSL.**B) United States****TSCA Status:** This product is not listed on the US EPA TSCA.**C) European Union****ECHA Status:** This product is not registered with the EU ECHA.**15.2 Chemical Safety Assessment**

No data available

**16. OTHER INFORMATION****16.1 Revision History**

Original Publication Date: 9/21/2015

**16.2 List of Abbreviations**

LD50	Median lethal dose of a substance required to kill 50% of a test population.
LC50	Medial lethal concentration of a substance required to kill 50% of a test population.
LDLo	Lowest known lethal dose
TDLo	Lowest known toxic dose
IARC	International Agency for Research on Cancer
NTP	National Toxicology Program
RTECS	Registry of Toxic Effects of Chemical Substances

**16.3 Further Information**

Copyright 2015. Toronto Research Chemicals Inc. Copies may be made for internal use only. The above information is believed to be correct to the best of our knowledge, but is to be only used as a guide. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Please take all due care when handling this product.