

## 1. PRODUCT AND COMPANY IDENTIFICATION

### 1.1 Product identifier

Product name : Theobromine-d<sub>3</sub>  
Catalog No. : HY-N0138S1  
CAS No. : 65566-69-0

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

Identified uses : Laboratory chemicals, manufacture of substances.

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

Company: MedChemExpress USA  
Tel: 609-228-6898  
Fax: 609-228-5909  
E-mail: sales@medchemexpress.com

### 1.4 Emergency telephone number

Emergency Phone #: 609-228-6898

## 2. HAZARDS IDENTIFICATION

### 2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

### 2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

### 2.3 Other hazards

None.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms: 3,7-Dimethylxanthine-d<sub>3</sub>  
Formula: C<sub>7</sub>H<sub>5</sub>D<sub>3</sub>N<sub>4</sub>O<sub>2</sub>  
Molecular Weight: 183.18  
CAS No. : 65566-69-0

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### Eye contact

Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water. Separate eyelids with fingers to ensure adequate flushing. Promptly call a physician.

#### Skin contact

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Rinse skin thoroughly with large amounts of water. Remove contaminated clothing and shoes and call a physician.

#### **Inhalation**

Immediately relocate self or casualty to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth-to-mouth resuscitation.

#### **Ingestion**

Wash out mouth with water; Do NOT induce vomiting; call a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2).

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

Treat symptomatically.

## **5. FIRE FIGHTING MEASURES**

### **5.1 Extinguishing media**

#### **Suitable extinguishing media**

Use water spray, dry chemical, foam, and carbon dioxide fire extinguisher.

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

During combustion, may emit irritant fumes.

### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus and protective clothing.

## **6. ACCIDENTAL RELEASE MEASURES**

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

Use full personal protective equipment. Avoid breathing vapors, mist, dust or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

Refer to protective measures listed in sections 8.

### **6.2 Environmental precautions**

Try to prevent further leakage or spillage. Keep the product away from drains or water courses.

### **6.3 Methods and materials for containment and cleaning up**

Absorb solutions with finely-powdered liquid-binding material (diatomite, universal binders); Decontaminate surfaces and equipment by scrubbing with alcohol; Dispose of contaminated material according to Section 13.

## **7. HANDLING AND STORAGE**

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

Avoid inhalation, contact with eyes and skin. Avoid dust and aerosol formation. Use only in areas with appropriate exhaust ventilation.

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

Keep container tightly sealed in cool, well-ventilated area. Keep away from direct sunlight and sources of ignition.

Recommended storage temperature:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month

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Shipping at room temperature if less than 2 weeks.

### 7.3 Specific end use(s)

No data available.

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

This product contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Engineering controls

Ensure adequate ventilation. Provide accessible safety shower and eye wash station.

#### Personal protective equipment

Eye protection	Safety goggles with side-shields.
Hand protection	Protective gloves.
Skin and body protection	Impervious clothing.
Respiratory protection	Suitable respirator.
Environmental exposure controls	Keep the product away from drains, water courses or the soil. Clean spillages in a safe way as soon as possible.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

Appearance	Solid
Odor	No data available
Odor threshold	No data available
pH	No data available
Melting/freezing point	No data available
Boiling point/range	No data available
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapor pressure	No data available
Vapor density	No data available
Relative density	No data available
Water Solubility	No data available
Partition coefficient	No data available
Auto-ignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### 9.2 Other safety information

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No data available.

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available.

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available.

### 10.4 Conditions to avoid

No data available.

### 10.5 Incompatible materials

Strong acids/alkalis, strong oxidising/reducing agents.

### 10.6 Hazardous decomposition products

Under fire conditions, may decompose and emit toxic fumes.

Other decomposition products - no data available.

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

Classified based on available data. For more details, see section 2

#### Skin corrosion/irritation

Classified based on available data. For more details, see section 2

#### Serious eye damage/irritation

Classified based on available data. For more details, see section 2

#### Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

#### Germ cell mutagenicity

Classified based on available data. For more details, see section 2

#### Carcinogenicity

IARC: No component of this product present at a level equal to or greater than 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by ACGIH.

NTP: No component of this product present at a level equal to or greater than 0.1% is identified as a anticipated or confirmed carcinogen by NTP.

OSHA: No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by OSHA.

#### Reproductive toxicity

Classified based on available data. For more details, see section 2

#### Specific target organ toxicity - single exposure

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Classified based on available data. For more details, see section 2

**Specific target organ toxicity - repeated exposure**

Classified based on available data. For more details, see section 2

**Aspiration hazard**

Classified based on available data. For more details, see section 2

**Additional information**

This information is based on our current knowledge. However the chemical, physical, and toxicological properties have not been completely investigated.

## 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

PBT/vPvB assessment unavailable as chemical safety assessment not required or not conducted.

### 12.6 Other adverse effects

No data available.

## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

Dispose substance in accordance with prevailing country, federal, state and local regulations.

**Contaminated packaging**

Conduct recycling or disposal in accordance with prevailing country, federal, state and local regulations.

## 14. TRANSPORT INFORMATION

**DOT (US)**

Proper shipping name: Not dangerous goods

UN number: -

Class: -

Packing group: -

**IMDG**

Proper shipping name: Not dangerous goods

UN number: -

Class: -

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Packing group: -

**IATA**

Proper shipping name: Not dangerous goods

UN number: -

Class: -

Packing group: -

## 15. REGULATORY INFORMATION

**SARA 302 Components:**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components:**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards:**

No SARA Hazards.

**Massachusetts Right To Know Components:**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components:**

No components are subject to the Pennsylvania Right to Know Act.

**New Jersey Right To Know Components:**

No components are subject to the New Jersey Right to Know Act.

**California Prop. 65 Components:**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or anyother reproductive harm.

## 16. OTHER INFORMATION

Copyright 2023 MedChemExpress. The above information is correct to the best of our present knowledge but does not purport to be all inclusive and should be used only as a guide. The product is for research use only and for experienced personnel. It must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The burden of safe use of this material rests entirely with the user. MedChemExpress disclaims all liability for any damage resulting from handling or from contact with this product.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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