

## SAFETY DATA SHEET

Revision Date 30-Mar-2024

Revision Number 3

### 1. Identification

**Product Name** Theophylline monohydrate

**Cat No. :** A15997

**CAS No** 5967-84-0  
**Synonyms** No information available

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

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

##### Company

Thermo Fisher Scientific Chemicals, Inc.  
30 Bond Street  
Ward Hill, MA 01835-8099  
Tel: 800-343-0660  
Fax: 800-322-4757

##### **Emergency Telephone Number**

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

### 2. Hazard(s) identification

#### **Classification**

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity

Category 3

#### Label Elements

##### **Signal Word**

Danger

##### **Hazard Statements**

Toxic if swallowed

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling  
Do not eat, drink or smoke when using this product

**Ingestion**

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
Rinse mouth

**Storage**

Store locked up

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

None identified

### 3. Composition/Information on Ingredients

Component	CAS No	Weight %
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate	5967-84-0	<=100

### 4. First-aid measures

<b>General Advice</b>	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
<b>Eye Contact</b>	In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Inhalation</b>	Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Most important symptoms and effects</b>	None reasonably foreseeable.
<b>Notes to Physician</b>	Treat symptomatically

### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Carbon dioxide (CO <sub>2</sub> ). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion.
<b>Unsuitable Extinguishing Media</b>	No information available

<b>Flash Point</b>	No information available
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	No information available
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

**Specific Hazards Arising from the Chemical**

Keep product and empty container away from heat and sources of ignition.

**Hazardous Combustion Products**

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</sub>).

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

**NFPA**

<b>Health</b>	<b>Flammability</b>	<b>Instability</b>	<b>Physical hazards</b>
3	1	0	-

**6. Accidental release measures**

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.
<b>Environmental Precautions</b>	Should not be released into the environment. See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up** Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

**7. Handling and storage**

<b>Handling</b>	Wear personal protective equipment/face protection. Avoid dust formation. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe (dust, vapor, mist, gas). Do not ingest. If swallowed then seek immediate medical assistance.
<b>Storage.</b>	Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Oxidizing agent.

**8. Exposure controls / personal protection**

<b>Exposure Guidelines</b>	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
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<b>Engineering Measures</b>	None under normal use conditions.
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**Personal Protective Equipment**

<b>Eye/face Protection</b>	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
<b>Skin and body protection</b>	Wear appropriate protective gloves and clothing to prevent skin exposure.

<b>Respiratory Protection</b>	No protective equipment is needed under normal use conditions.
<b>Recommended Filter type:</b>	Particle filter.
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

<b>Physical State</b>	Solid
<b>Appearance</b>	White
<b>Odor</b>	Odorless
<b>Odor Threshold</b>	No information available
<b>pH</b>	No information available
<b>Melting Point/Range</b>	270 - 274 °C / 518 - 525.2 °F
<b>Boiling Point/Range</b>	No information available
<b>Flash Point</b>	No information available
<b>Evaporation Rate</b>	Not applicable
<b>Flammability (solid,gas)</b>	No information available
<b>Flammability or explosive limits</b>	
Upper	No data available
Lower	No data available
<b>Vapor Pressure</b>	No information available
<b>Vapor Density</b>	Not applicable
<b>Specific Gravity</b>	No information available
<b>Solubility</b>	No information available
<b>Partition coefficient; n-octanol/water</b>	No data available
<b>Autoignition Temperature</b>	No information available
<b>Decomposition Temperature</b>	No information available
<b>Viscosity</b>	Not applicable
<b>Molecular Formula</b>	C7 H8 N4 O2.H2 O
<b>Molecular Weight</b>	198.18 (180.16anhy)

## 10. Stability and reactivity

<b>Reactive Hazard</b>	None known, based on information available
<b>Stability</b>	Stable under normal conditions.
<b>Conditions to Avoid</b>	Incompatible products.
<b>Incompatible Materials</b>	Oxidizing agent
<b>Hazardous Decomposition Products</b>	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Nitrogen oxides (NO <sub>x</sub> )
<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

### Acute Toxicity

#### Product Information

#### Component Information

<b>Toxicologically Synergistic Products</b>	No information available
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### Delayed and immediate effects as well as chronic effects from short and long-term exposure

<b>Irritation</b>	No information available
<b>Sensitization</b>	No information available

**Carcinogenicity**

The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate	5967-84-0	Not listed	Not listed	Not listed	Not listed	Not listed

**Mutagenic Effects**

No information available

**Reproductive Effects**

No information available.

**Developmental Effects**

No information available.

**Teratogenicity**

No information available.

**STOT - single exposure**

None known

**STOT - repeated exposure**

None known

**Aspiration hazard**

No information available

**Symptoms / effects, both acute and delayed**

No information available

**Endocrine Disruptor Information**

No information available

**Other Adverse Effects**

The toxicological properties have not been fully investigated.

## 12. Ecological information

**Ecotoxicity**

Do not empty into drains.

**Persistence and Degradability**

No information available

**Bioaccumulation/ Accumulation**

No information available.

**Mobility**

No information available.

## 13. Disposal considerations

**Waste Disposal Methods**

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## 14. Transport information

**DOT****UN-No**

UN2811

**Proper Shipping Name**

Toxic solid, organic, n.o.s.

**Technical Name**

(Theophylline monohydrate)

**Hazard Class**

6.1

**Packing Group**

III

**TDG****UN-No**

UN2811

**Proper Shipping Name**

Toxic solid, organic, n.o.s.

**Hazard Class**

6.1

**Packing Group**

III

**IATA****UN-No**

UN2811

**Proper Shipping Name**

TOXIC SOLID, ORGANIC, N.O.S.\*

**Hazard Class**

6.1

**Packing Group**

III

**IMDG/IMO**

<b>UN-No</b>	UN2811
<b>Proper Shipping Name</b>	Toxic solid, organic, n.o.s.
<b>Hazard Class</b>	6.1
<b>Packing Group</b>	III

**15. Regulatory information****United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate	5967-84-0	-	-	-

**Legend:****TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)**

Not applicable

**TSCA 12(b)** - Notices of Export

Not applicable

**International Inventories**

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate	5967-84-0	-	-	-	-	-		X	-	-

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)**U.S. Federal Regulations****SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

**SARA 311/312 Hazard Categories**

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

**CWA (Clean Water Act)**

Not applicable

**Clean Air Act**

Not applicable

**OSHA** - Occupational Safety and Health Administration

Not applicable

**CERCLA**

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

**California Proposition 65** This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations** Not applicable

**U.S. Department of Transportation**

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** No information available

**Authorisation/Restrictions according to EU REACH** Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate	5967-84-0	-	-	-

**Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate	5967-84-0	Not applicable	Not applicable	Not applicable	Not applicable

**Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?**

Not applicable

**Other International Regulations**

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate	5967-84-0	Not applicable	Not applicable	Not applicable	Not applicable

**16. Other information**

**Prepared By** Health, Safety and Environmental Department  
Email: chem.techinfo@thermofisher.com

www.thermofisher.com

<b>Revision Date</b>	30-Mar-2024
<b>Print Date</b>	30-Mar-2024
<b>Revision Summary</b>	New emergency telephone response service provider.

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of SDS**