

## SAFETY DATA SHEET

Creation Date 22-September-2009

Revision Date 19-February-2020

Revision Number 4

### 1. Identification

**Product Name** Theophylline

**Cat No. :** AC250310000; AC250310010; AC250310050; AC250312500

**CAS-No** 58-55-9

**Synonyms** 3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione; 1,3-Dimethylxanthine; 1,3-Dimethyl-2,6-dioxo-1,2,3,6-tetrahydropurine

**Recommended Use** Laboratory chemicals.

**Uses advised against** Food, drug, pesticide or biocidal product use.

**Details of the supplier of the safety data sheet**

#### Company

**Importer/Distributor**  
Fisher Scientific  
112 Colonnade Road,  
Ottawa, ON K2E 7L6,  
Canada  
Tel: 1-800-234-7437

Acros Organics  
One Reagent Lane  
Fair Lawn, NJ 07410

#### **Manufacturer**

Fisher Scientific  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

#### **Emergency Telephone Number**

For information **US** call: 001-800-ACROS-01 / **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

**WHMIS 2015 Classification** Classified as hazardous under the Hazardous Products Regulations (SOR/2015-17)

**Acute oral toxicity** Category 3

#### Label Elements

#### **Signal Word**

Danger

#### **Hazard Statements**

Toxic if swallowed

**Precautionary Statements****Manufacturer**

Alfa Aesar  
 Thermo Fisher Scientific Chemicals, Inc.  
 30 Bond Street, Ward Hill, MA 01835-8099  
**Tel:** 800-343-0660 **Fax:** 800-322-4757  
**Email:** tech@alfa.com  
**www.alfa.com**

**Prevention**

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

**Response**

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

**Storage**

Store locked up

**Disposal**

Dispose of contents/container to an approved waste disposal plant

### 3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Theophylline	58-55-9	<=100

### 4. First-aid measures

**General Advice**

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

**Eye Contact**

In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

**Inhalation**

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.

**Ingestion**

Do NOT induce vomiting. Call a physician or poison control center immediately.

**Most important symptoms/effects**  
**Notes to Physician**

No information available.  
 Treat symptomatically

### 5. Fire-fighting measures

**Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam.

<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>	Not applicable
<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**

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

**Health**  
3

**Flammability**  
1

**Instability**  
0

**Physical hazards**  
N/A

## 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.

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

## 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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**Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

**Personal protective equipment**

<b>Eye 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
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**Hand Protection** EN166.  
Protective gloves

Glove material	Breakthrough time	Glove thickness	Glove comments
Nitrile rubber Neoprene Natural rubber PVC	See manufacturers recommendations	-	Splash protection only

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

#### Respiratory Protection

No protective equipment is needed under normal use conditions.

#### Environmental exposure controls

No information available.

#### Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

## 9. Physical and chemical properties

<b>Physical State</b>	Powder Solid
<b>Appearance</b>	White
<b>Odor</b>	Odorless
<b>Odor Threshold</b>	No information available
<b>pH</b>	5 - 8 g/l aq.sol
<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>	
<b>Upper</b>	No data available
<b>Lower</b>	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>	Soluble in water
<b>Partition coefficient; n-octanol/water</b>	No data available
<b>Autoignition Temperature</b>	Not applicable
<b>Decomposition Temperature</b>	No information available
<b>Viscosity</b>	Not applicable
<b>Molecular Formula</b>	C7 H8 N4 O2
<b>Molecular Weight</b>	180.17

## 10. Stability and reactivity

<b>Reactive Hazard</b>	None known, based on information available
<b>Stability</b>	No information available.
<b>Conditions to Avoid</b>	Incompatible products.

<b>Incompatible Materials</b>	Strong oxidizing agents
<b>Hazardous Decomposition Products</b>	Nitrogen oxides (NO <sub>x</sub> ), Carbon monoxide (CO), Carbon dioxide (CO <sub>2</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** The toxicological properties have not been fully investigated

#### **Component Information**

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Theophylline	LD50 = 225 mg/kg ( Rat )	LD50 > 2000 mg/kg ( Rabbit )	LC50 > 6.7 mg/L ( Rat ) 4 h

**Toxicologically Synergistic Products** No information available

### Delayed and immediate effects as well as chronic effects from short and long-term exposure

**Irritation** No information available

**Sensitization** 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
Theophylline	58-55-9	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** Soluble in water Persistence is unlikely based on information available.

**Bioaccumulation/ Accumulation** No information available.

**Mobility** Will likely be mobile in the environment due to its water solubility.

### 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 SOLIDS, ORGANIC, N.O.S.  
**Technical Name** Theophylline  
**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**

**UN-No** UN2811  
**Proper Shipping Name** TOXIC SOLID, ORGANIC, N.O.S.  
**Hazard Class** 6.1  
**Packing Group** III

### 15. Regulatory information

**International Inventories**

Component	DSL	NDSL	TSCA	EINECS	ELINCS	PICCS	ENCS	AICS	KECL	IECSC
Theophylline	X	-	X	200-385-7	-	X	X	X	KE-10629	X

**Legend**

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**Canada**

SDS in compliance with provisions of information as set out in Canadian Standard - Part 4, Schedule 1 and 2 of the Hazardous Products Regulations (HPR) and meets the requirements of the HPR (Paragraph 13(1)(a) of the Hazardous Products Act (HPA)).

### 16. Other information

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19-February-2020

**Revision Summary**

This document has been updated to comply with the requirements of WHMIS 2015 to align with the Globally Harmonised System (GHS) for the Classification and Labelling of Chemicals.

**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**