

SAFETY DATA SHEET

Creation Date 22-Sep-2009

Revision Date 19-Dec-2025

Revision Number 7

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

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

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

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

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 according to [US] OSHA (29 CFR 1910.1200, 2024)

Acute oral toxicity
Reproductive Toxicity

Category 3
Category 1B

Label Elements

Signal Word

Danger

Hazard Statements

Toxic if swallowed
May damage the unborn child

**Precautionary Statements****Prevention**

Obtain special instructions before use
Do not handle until all safety precautions have been read and understood
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection

Response

IF exposed or concerned: Get medical attention/advice

Ingestion

IF SWALLOWED: Immediately call a POISON CENTER or doctor

Rinse mouth

Storage

Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

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 and effects

None reasonably foreseeable.

Notes to Physician

Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam.

Unsuitable Extinguishing Media No information available

Flash Point No information available
Method - No information available

Autoignition Temperature Not applicable

Explosion Limits

Upper No data available

Lower No data available

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge 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_x). Carbon monoxide (CO). Carbon dioxide (CO₂).

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

Personal Precautions 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.

Environmental Precautions 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

Handling 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.

Storage. Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

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

Personal Protective Equipment

Eye/face Protection	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.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	No protective equipment is needed under normal use conditions.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State	Powder Solid
Color	White
Odor	Odorless
Odor Threshold	No information available

Property

<u>Values</u>	<u>Remarks</u>	<u>• Method</u>
Melting Point/Range	270 - 274 °C / 518 - 525.2 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flash Point	No information available	Method - No information available
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Autoignition Temperature	Not applicable	
Decomposition Temperature	No data available	
pH	5	8 g/l aq.sol
Viscosity	Not applicable	Solid
Water Solubility	8.3 g/l (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Theophylline	-0.008	
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

Other Information

Molecular Formula	C7 H8 N4 O2
Molecular Weight	180.17
Evaporation Rate	Not applicable - Solid

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	No information available.
Conditions to Avoid	Incompatible products.
Incompatible Materials	Strong oxidizing agents

Hazardous Decomposition Products Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂)

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation Avoid breathing dust or spray mist. May be harmful if inhaled.
Ingestion May be harmful if swallowed.
Eyes Avoid contact with eyes.
Skin Avoid contact with skin.

Toxicology data for the components

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

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;
Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) 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

(g) reproductive toxicity; Category 1B

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs None known.

(j) aspiration hazard; Solid
Not applicable

Other Adverse Effects

Symptoms / effects, both acute and No information available.

delayed

Other Adverse Effects .

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

Do not empty into drains. .

Persistence and Degradability Persistence is unlikely

Bioaccumulation/ Accumulation No information available.

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

Component	log Pow
Theophylline	-0.008

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 Shipping Name Theophylline
 Hazard Class 6.1
 Packing Group III

TDG

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

IATA

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

IMDG/IMO

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

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Theophylline	58-55-9	X	ACTIVE	-

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

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Theophylline	58-55-9	X	-	200-385-7	X	X		X	X	KE-10629

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)
Theophylline	58-55-9	-	Use restricted. See entry 30. (see link for restriction details) Use restricted. See entry 75. (see link for restriction details)	-

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)
Theophylline	58-55-9	Listed	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)
Theophylline	58-55-9	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By

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Revision Summary

Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

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