

SAFETY DATA SHEET

Creation Date 22-Sep-2009

Revision Date 31-Aug-2023

Revision Number 6

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 NumberFor information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11Emergency 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
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
Use personal protective equipment as required
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product

Response

IF exposed or concerned: Get medical attention/advice

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 %
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 (CO ₂). 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

Physical State	Powder Solid
Appearance	White
Odor	Odorless
Odor Threshold	No information available
pH	5 - 8 g/l aq.sol
Melting Point/Range	270 - 274 °C / 518 - 525.2 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	Soluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	Not applicable
Decomposition Temperature	No information available
Viscosity	Not applicable
Molecular Formula	C7 H8 N4 O2
Molecular Weight	180.17

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 (NOx), Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information 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 .

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 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**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** Not applicable**SARA 311/312 Hazard Categories** See section 2 for more information**CWA (Clean Water Act)** Not applicable**Clean Air Act** Not applicable**OSHA** - Occupational Safety and Health Administration Not applicable**CERCLA** Not applicable**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	-	-	-

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 Regulatory Affairs
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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