

SAFETY DATA SHEET

Creation Date 22-September-2009

Revision Date 26-March-2024

Revision Number 5

1. Identification

Product Name Theophylline

Cat No. : J60203

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

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****WHMIS 2015 Classification**

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

Acute oral toxicity	Category 3
Reproductive Toxicity	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 SWALLOWED: Immediately call a POISON CENTER/doctor
IF exposed or concerned: Get medical advice/attention
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	None reasonably foreseeable. 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

<u>Exposure Guidelines</u>	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
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<u>Engineering Measures</u>	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
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Personal protective equipment

Eye 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.
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Hand Protection

Protective gloves

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

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

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 (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂)

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

International Inventories

Component	CAS-No	DSL	NDSL	TSCA	TSCA Inventory notification - Active-Inactive	EINECS	ELINCS	NLP
Theophylline	58-55-9	X	-	X	ACTIVE	200-385-7	-	-

Component	CAS-No	IECSC	KECL	ENCS	ISHL	TCSI	AICS	NZIoC	PICCS
Theophylline	58-55-9	X	KE-10629	X	-	X	X	X	X

Legend:

X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

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

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

PICCS - Philippines Inventory of Chemicals and 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)).

Other International Regulations

Authorisation/Restrictions according to EU REACH

Not applicable

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

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

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Creation Date

22-September-2009

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26-March-2024

Print Date

26-March-2024

Revision Summary

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