SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name	:	Theophylline (200 mg)
Product Number	:	1653004
Brand	:	US Pharmacopeia
Index-No.	:	613-342-00-6
CAS-No.	:	58-55-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	:	Laboratory chemicals, Synthesis of substances
Restrictions on use	:	The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company	:	Sigma-Aldrich Inc. SPRUCE ST 3050 63103 St. Louis Telephone :(314) 771-5765 Telefax: (800) 325-5052

1.4 Emergency telephone number

Emergency Phone #	:	800 424 9300 (CHEMTREC) 24/7 +1 703 527 3887 (CHEMTREC) 24/7

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SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Acute toxicity (Oral) : Category 3

Reproductive toxicity : Category 1B

Other hazards

None known.

GHS label elements

Hazard pictograms :

Signal word : Danger

Hazard statements : H301 Toxic if swallowed.
H360 May damage fertility or the unborn child.

Precautionary statements :

Prevention:

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.

Storage:

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

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CAS-No. : 58-55-9

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Theophylline	58-55-9*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.
TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Call in physician.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact : After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed : If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media : Water
Foam
Carbon dioxide (CO2)

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Dry powder

Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	:	Carbon oxides Nitrogen oxides (NOx)
Specific extinguishing methods	:	No data available
Further information	:	Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: Wear appropriate personal protective equipment, as indicated in Section 8.
Environmental precautions	:	Do not let product enter drains.

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Methods and materials for containment and cleaning up	:	Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements

Advice on safe handling	:	Work under hood. Do not inhale substance/mixture.
Further information on storage conditions	:	Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.
Storage class	:	6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects
Recommended storage temperature	:	Recommended storage temperature if relevant, see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures	:	No data available

Personal protective equipment

Respiratory protection	:	required when dusts are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.
Recommended Filter type:	:	Filter type P3

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The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0.11 mm
Protective index	:	Full contact
Manufacturer	:	KCL 741 Dermatril® L

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0.11 mm
Protective index	:	Splash contact
Manufacturer	:	KCL 741 Dermatril® L

Remarks	:	Handle with impervious gloves. This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	:	protective clothing
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	powder
Colour	:	white

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Odour	:	odourless
Odour Threshold	:	Not applicable
pH	:	No data available
Melting point/ range	:	525 - 527 °F / 274 - 275 °C
Boiling point/boiling range	:	No data available
Flash point	:	Not applicable
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Self-ignition	:	1130 °F / 610 °C 1,013 hPa
Upper explosion limit / Upper flammability limit	:	No data available
Lower explosion limit / Lower flammability limit	:	No data available
Vapour pressure	:	No data available
Relative vapour density	:	No data available
Relative density	:	No data available
Density	:	1.36 g/cm3 (77 °F / 25 °C)
Solubility(ies) Water solubility	:	5.5 g/l (67.8 °F / 19.9 °C)
Partition coefficient: n-octanol/water	:	log Pow: -0.008 (73 °F / 23 °C) Bioaccumulation is not expected.
Autoignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, dynamic	:	No data available

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Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Molecular weight	:	180.16 g/mol
Particle characteristics Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	Violent reactions possible with: Strong oxidizing agents
Conditions to avoid	:	no information available
Incompatible materials	:	No data available
Hazardous decomposition products	:	For Hazardous combustion products in the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 225 mg/kg
Remarks: (RTECS)
LC50 Inhalation - Rat - male and female - 4 h - > 6.7 mg/l - aerosol

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(OECD Test Guideline 403)
LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)
Remarks: The value is given in analogy to the following substances: Caffeine

Germ cell mutagenicity
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA)
Test Type: Chromosome aberration test in vitro
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 473
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative

Test Type: Micronucleus test
Species: Mouse
Cell type: Red blood cells (erythrocytes)
Application Route: Oral

Result: negative
Remarks: (ECHA)

Test Type: Chromosome aberration test
Species: Rat
Cell type: sperm
Application Route: Oral

Result: negative
Remarks: (ECHA)

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Test Type: Chromosome aberration test
Species: Mouse
Cell type: Bone marrow
Application Route: Intraperitoneal

Result: negative
Remarks: (ECHA)

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
May damage the unborn child.

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 13 Weeks - Lowest observed adverse effect level - 37.5 mg/kg
Remarks: (ECHA)

Nausea, Vomiting, Headache, Diarrhoea, Epigastric pain., Circulatory collapse
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Theophylline:

Toxicity to fish	:	LC50 (Leuciscus idus (Golden orfe)): 100 mg/l Exposure time: 96 h

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Test Type: static test
Method: DIN 38412 part 15

Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 178 mg/l Exposure time: 48 h Test Type: static test Method: Directive 67/548/EEC, Annex V, C.2.
Toxicity to algae/aquatic plants	:	ErC50 (Desmodesmus subspicatus (green algae)): > 100 mg/l Exposure time: 72 h Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes
Toxicity to microorganisms	:	EC50 (activated sludge): > 1,000 mg/l Exposure time: 3 h Method: OECD Test Guideline 209 GLP: yes

Persistence and degradability

Components:

Theophylline:

Biodegradability	:	aerobic Inoculum: activated sludge Concentration: 43 mg/l Result: Readily biodegradable. Biodegradation: > 90 - 100 % Exposure time: 22 d Method: OECD Test Guideline 301A GLP: yes

Bioaccumulative potential

Components:

Theophylline:

Partition coefficient: n-octanol/water	:	log Pow: -0.008 (73 °F / 23 °C) Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential	:	Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances

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Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues	:	Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No.	:	UN 2811
Proper shipping name	:	Toxic solid, organic, n.o.s. (Theophylline)
Class	:	6.1
Packing group	:	III
Labels	:	Division 6.1 - Toxic substances
Packing instruction (cargo aircraft)	:	677
Packing instruction (passenger aircraft)	:	670

IMDG-Code

UN number	:	UN 2811
Proper shipping name	:	TOXIC SOLID, ORGANIC, N.O.S. (Theophylline)
Class	:	6.1
Packing group	:	III
Labels	:	6.1
EmS Code	:	F-A, S-A
Marine pollutant	:	no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number	:	UN 2811
Proper shipping name	:	Toxic solids, organic, n.o.s.

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(Theophylline)

Class	:	6.1
Packing group	:	III
Labels	:	Division 6.1 - Toxic substances
ERG Code	:	154
Marine pollutant	:	no
Poison Inhalation Hazard	:	No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards	:	Acute Health Hazard Chronic Health Hazard
SARA 313	:	This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).
This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. Clean Water Act, Section 311, Table 116.4A.
This product does not contain any Hazardous Chemicals listed under the U.S. Clean Water Act, Section 311, Table 117.3.

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This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307
This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

US TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); LSPN - List of Hazardous Notified Substances (Chile); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire

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Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
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Revision Date : 08/11/2026

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