

SAFETY DATA SHEET

Version 6.9
Revision Date 08/05/2024
Print Date 08/06/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Theophylline

Product Number : T1633

Brand : Sigma

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

Uses advised against : 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.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 3), H301
Reproductive toxicity (Category 1B), H360

For the full text of the H-Statements mentioned in this Section, see Section 16.

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2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H301

Toxic if swallowed.

H360

May damage fertility or the unborn child.

Precautionary Statements

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.

P301 + P310 + P330

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

P308 + P313

IF exposed or concerned: Get medical advice/ attention.

P405

Store locked up.

P501

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

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms

: 1,3-Dimethylxanthine
3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione
2,6-Dihydroxy-1,3-dimethylpurine

Formula

: C₇H₈N₄O₂

Molecular weight

: 180.16 g/mol

CAS-No.

: 58-55-9

EC-No.

: 200-385-7

Index-No.

: 613-342-00-6

Component	Classification	Concentration
Theophylline	Acute Tox. 3; Repr. 1B; H301, H360	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

No data available

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

No data available

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Nitrogen oxides (NO_x)
Combustible.

5.3 Advice for firefighters

No data available

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.

6.2 Environmental precautions

No data available

6.3 Methods and materials for containment and cleaning up

No data available

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

No data available

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

No data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: powder
Color: white |
| b) Odor | odorless |
| c) Odor Threshold | Not applicable |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/ range: 274 - 275 °C (525 - 527 °F) |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | ()Not applicable |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapor pressure | No data available |
| l) Vapor density | No data available |
| m) Density | 1.36 g/cm ³ at 25 °C (77 °F) |
| Relative density | No data available |
| n) Water solubility | 5.5 g/l at 19.9 °C (67.8 °F) |
| o) Partition coefficient: n-octanol/water | log Pow: -0.008 at 23 °C (73 °F) - Bioaccumulation is not expected. |
| p) Autoignition temperature | 610 °C (1130 °F) at 1,013 hPa |
| q) Decomposition temperature | No data available |

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- r) Viscosity No data available
s) Explosive properties No data available
t) Oxidizing properties none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

No data available

10.3 Possibility of hazardous reactions

Violent reactions possible with:
Strong oxidizing agents

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition 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

(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

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(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)

Test Type: Chromosome aberration test

Species: Mouse

Cell type: Bone marrow

Application Route: Intraperitoneal

Result: negative

Remarks: (ECHA)

Carcinogenicity

IARC: No ingredient 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 ingredient 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 - LOAEL (Lowest observed adverse effect level) - 37.5 mg/kg

Remarks: (ECHA)

RTECS: XH3850000

Nausea, Vomiting, Headache, Diarrhea, 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

12.1 Toxicity

Toxicity to fish	static test LC50 - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h (DIN 38412 part 15)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 178 mg/l - 48 h (Directive 67/548/EEC, Annex V, C.2.)
Toxicity to algae	ErC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 22 d Result: > 90 - 100 % - Readily biodegradable. (OECD Test Guideline 301A)
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

DOT (US)

UN number: 2811 Class: 6.1 Packing group: III
Proper shipping name: Toxic solids, organic, n.o.s. (Theophylline)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2811 Class: 6.1 Packing group: III EMS-
No: F-A, S-A
Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (Theophylline)

IATA

UN number: 2811 Class: 6.1 Packing group: III
Proper shipping name: Toxic solid, organic, n.o.s. (Theophylline)

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 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.

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 ingredients of this product are reported in the following inventories:

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

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

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