

## SAFETY DATA SHEET

Version 6.4  
Revision Date 12/18/2020  
Print Date 06/10/2023

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Theophylline

Product Number : T1633  
Brand : Sigma  
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

**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

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

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word : Danger

Hazard statement(s)  
H301 : Toxic if swallowed.

Precautionary statement(s)  
P264 : Wash skin thoroughly after handling.

Sigma - T1633

Page 1 of 9

P270	Do not eat, drink or smoke when using this product.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
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	: C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub>
Molecular weight	: 180.16 g/mol
CAS-No.	: 58-55-9
EC-No.	: 200-385-7

Component	Classification	Concentration
<b>Theophylline</b>		
	Acute Tox. 3; H301	<= 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

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air.

#### In case of skin contact

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

#### In case of eye contact

After eye contact: rinse out with plenty of water. 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.

### 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**

##### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

##### **Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

#### **5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

#### **5.3 Advice for firefighters**

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

#### **5.4 Further information**

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

### **SECTION 6: Accidental release measures**

#### **6.1 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.

For personal protection see section 8.

#### **6.2 Environmental precautions**

Do not let product enter drains.

#### **6.3 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.

#### **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**

##### **Storage conditions**

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

### 7.3 Specific end use(s)

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

---

## 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

#### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### Skin protection

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatrill® L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatrill® L

##### Body Protection

protective clothing

##### 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.

##### Control of environmental exposure

Do not let product enter drains.

---

## 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	No data available
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	( )No data available
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) Relative density	1.35 g/cm <sup>3</sup> at 25 °C (77 °F)
n) Water solubility	5.5 g/l at 19.9 °C (67.8 °F)
o) Partition coefficient: n-octanol/water	log Pow: -0.007 at 23 °C (73 °F)
p) Autoignition temperature	610 °C (1130 °F) at 1,013 hPa
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

### 9.2 Other safety information

No data available

---

## SECTION 10: Stability and reactivity

### 10.1 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.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Sigma - T1633

Page 5 of 9

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Strong oxidizing agents

### 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  
(OECD Test Guideline 403)

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

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Mouse

lymphocyte

Result: negative

Mouse - male and female

Result: negative

#### 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

No data available

No data available

**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**

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	LC50 - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h (DIN 38412)
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	EC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)

**12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 22 d  
Result: 90 - 100 % - Readily biodegradable.

**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 Other adverse effects**

No data available

---

**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Product**

Waste material must be disposed of in accordance with the national and local No mixing with other waste. Handle uncleaned containers like the product See

---

## 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

### SARA 302 Components

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

### SARA 313 Components

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.

### Massachusetts Right To Know Components

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

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

### Pennsylvania Right To Know Components

Theophylline	CAS-No. 58-55-9	Revision Date
--------------	--------------------	---------------

### New Jersey Right To Know Components

Theophylline	CAS-No. 58-55-9	Revision Date
--------------	--------------------	---------------

---

## SECTION 16: Other information

### Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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](mailto:mlsbranding@sial.com).

Version: 6.4

Revision Date: 12/18/2020

Print Date: 06/10/2023