SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: Theophylline

Product Number: T1633
Brand: Sigma
REACH No.: A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.: 58-55-9

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

Identified uses: Laboratory chemicals, Manufacture 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

Classification according to Regulation (EC) No 1272/2008
Acute toxicity, Oral (Category 3), H301

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008
Pictogram

Signal word Danger
The life science business of Merck operates as MilliporeSigma in the US and Canada.

Hazard statement(s)
H301 Toxic if swallowed.

Precautionary statement(s)
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

Supplemental Hazard Statements none

2.3 Other hazards
This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

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\text{7}H\text{8}N\text{4}O\text{2}

Molecular weight: 180,16 g/mol

CAS-No.: 58-55-9

EC-No.: 200-385-7

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theophylline</td>
<td>Acute Tox. 3; H301</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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 (CO2) 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 (NOx)
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.

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

8.2 Exposure controls

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).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® 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.
Recommended Filter type: Filter type P3
The entrepreneur 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.

**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

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>a)</strong> Appearance</td>
<td>Form: powder</td>
</tr>
<tr>
<td>Color</td>
<td>white</td>
</tr>
<tr>
<td><strong>b)</strong> Odor</td>
<td>odorless</td>
</tr>
<tr>
<td><strong>c)</strong> Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>d)</strong> pH</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>e)</strong> Melting point/freezing point</td>
<td>Melting point/range: 274 - 275 °C</td>
</tr>
<tr>
<td><strong>f)</strong> Initial boiling point and boiling range</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>g)</strong> Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>h)</strong> Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>i)</strong> Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>j)</strong> Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>k)</strong> Vapor pressure</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>l)</strong> Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>m)</strong> Relative density</td>
<td>1,35 g/cm³ at 25 °C</td>
</tr>
<tr>
<td><strong>n)</strong> Water solubility</td>
<td>5,5 g/l at 19,9 °C</td>
</tr>
<tr>
<td><strong>o)</strong> Partition coefficient: n-octanol/water</td>
<td>log Pow: -0,007 at 23 °C</td>
</tr>
<tr>
<td><strong>p)</strong> Autoignition temperature</td>
<td>610 °C</td>
</tr>
<tr>
<td></td>
<td>at 1.013 hPa</td>
</tr>
<tr>
<td><strong>q)</strong> Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>r)</strong> Viscosity</td>
<td>Viscosity, kinematic: No data available</td>
</tr>
<tr>
<td></td>
<td>Viscosity, dynamic: No data available</td>
</tr>
<tr>
<td><strong>s)</strong> Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td><strong>t)</strong> Oxidizing properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

#### 9.2 Other safety information

No data available

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*The life science business of Merck operates as MilliporeSigma in the US and Canada*
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).

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)

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.
Reproductive toxicity
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.

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
This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Other adverse effects
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.
SECTION 14: Transport information

14.1 UN number
ADR/RID: 2811  
IMDG: 2811  
IATA: 2811

14.2 UN proper shipping name
ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (Theophylline)  
IMDG: TOXIC SOLID, ORGANIC, N.O.S. (Theophylline)  
IATA: Toxic solid, organic, n.o.s. (Theophylline)

14.3 Transport hazard class(es)
ADR/RID: 6.1  
IMDG: 6.1  
IATA: 6.1

14.4 Packaging group
ADR/RID: III  
IMDG: III  
IATA: III

14.5 Environmental hazards
ADR/RID: no  
IMDG Marine pollutant: no  
IATA: no

14.6 Special precautions for user
No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture
This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National legislation
H2 ACUTE TOXIC

Other regulations
Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment
For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.
H301 Toxic if swallowed.

Relevant changes since previous version
2. Hazards identification
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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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