

# SAFETY DATA SHEET

## 1. PRODUCT

### 1.1 Product identifiers

Name: Theophylline

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

## 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. P270 Do not eat, drink or smoke when using this product. P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. 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

No data available

## 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:  $C_7H_8N_4O_2$

Molecular weight: 180.16 g/mol

CAS-No.: 58-55-9

EC-No.: 200-385-7

#### Hazardous components

Component	Classification	Concentration
Theophylline	Acute Tox. 3; H301	<= 100 %

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

<b>General advice</b>
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
<b>If inhaled</b>
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
<b>In case of skin contact</b>
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.
<b>In case of eye contact</b>
Flush eyes with water as a precaution.
<b>If swallowed</b>
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 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

### 4.2 Indication of any immediate medical attention and special treatment needed

No data available

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

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

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.

Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

## 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

## 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Keep in a dry place.

Storage class (TRGS 510): Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

## 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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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### Personal protective equipment

Eye/face protection	Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Skin protection	Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. Full contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M) Splash contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M) data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374 If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.
Body Protection	Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
Respiratory protection	Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).
Control of environmental exposure	Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

## 9.1 Information on basic physical and chemical properties

Appearance	Form: powder Colour: white
Odour	odourless
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 274 - 275 °C (525 - 527 °F)
Initial boiling point and boiling range	No data available
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	1.35 g/cm <sup>3</sup> at 25 °C (77 °F)
Water solubility	5.5 g/l at 19.9 °C (67.8 °F)
Partition coefficient: n-octanol/water	log Pow: -0.007 at 23 °C (73 °F)
Auto-ignition temperature	610 °C (1,130 °F) at 1,013 hPa (760 mmHg)
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

## 9.2 Other safety information

No data available

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Other decomposition products - No data available

In the event of fire: see section 5

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

Acute toxicity
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LD50 Oral - Rat - female - 272 mg/kg 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
<b>Skin corrosion/irritation</b>
Skin - Rabbit Result: No skin irritation (OECD Test Guideline 404)
<b>Serious eye damage/eye irritation</b>
Eyes - Rabbit Result: No eye irritation (OECD Test Guideline 405)
<b>Respiratory or skin sensitisation</b>
No data available
<b>Germ cell mutagenicity</b>
Mouse lymphocyte Result: negative Mouse - male and female Result: negative
<b>Carcinogenicity</b>
IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Theophylline) ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH. 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 identified as a carcinogen or potential carcinogen by OSHA.
<b>Reproductive toxicity</b>
No data available No data available
<b>Specific target organ toxicity -single exposure</b>
No data available
<b>Specific target organ toxicity -repeated exposure</b>
No data available
<b>Aspiration hazard</b>
No data available
<b>Additional Information</b>
RTECS: XH3850000 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

## 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)
Toxicity to bacteria	No data available

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 22 d Result: 90 - 100 % - Readily biodegradable
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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 Other adverse effects

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.
Contaminated packaging
Dispose of as unused product.

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## 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)

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## 15. REGULATORY INFORMATION

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### 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.

### Pennsylvania Right To Know Components

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

### New Jersey Right To Know Components

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

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity

H301 Toxic if swallowed.

### HMIS Rating

Health hazard: 2

Chronic Health Hazard: \*

Flammability: 0

Physical Hazard 0

### NFPA Rating

Health hazard: 2

Fire Hazard: 0

Reactivity Hazard: 0

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