

## Chemical Safety Data Sheet MSDS / SDS

## Theophylline

Revision Date:2026-05-31 Revision Number:1

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

**Product identifier**

Product name : Theophylline  
CBnumber : CB4285388  
CAS : 58-55-9  
EINECS Number : 200-385-7  
Synonyms : Theophylline,theophylline

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

## SECTION 2: Hazards identification

**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

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 or doctor/physician.  
P405 Store locked up.  
P501 Dispose of contents/container to.....

**Hazard statements**

H301 Toxic if swallowed

## SECTION 3: Composition/information on ingredients

## Substance

|              |                             |
|--------------|-----------------------------|
| Product name | : Theophylline              |
| Synonyms     | : Theophylline,theophylline |
| CAS          | : 58-55-9                   |
| EC number    | : 200-385-7                 |
| MF           | : C7H8N4O2                  |
| MW           | : 180.16                    |

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### In case of skin contact

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

#### In case of eye contact

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

#### If swallowed

After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour).

### 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) and/or in section 11

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

No data available

### 4.4 Notes to physician

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

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

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

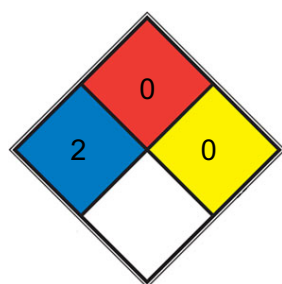
Forms explosive mixtures with air at ambient temperatures.

### 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.

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

### NFPA 704



**HEALTH 2** Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

**FIRE 0** Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,[N2](#))

**SPEC.**

**HAZ.**

## SECTION 6: Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

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. Risk of explosion.

### 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 with liquid-absorbent material (e.g.

Chemizorb®). Dispose of properly. Clean up affected area.

## 6.4 Reference to other sections

For disposal see section 13.

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# SECTION 7: Handling and storage

## 7.1 Precautions for safe handling

### Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

### Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

## 7.2 Conditions for safe storage, including any incompatibilities

### Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

### Storage stability Recommended storage temperature

2 - 8 °C

### Storage class

Storage class (TRGS 510): 3: Flammable liquids

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# SECTION 8: Exposure controls/personal protection

## 8.1 Control parameters

### Ingredients with workplace control parameters

|  |   |   |   |                              |
|--|---|---|---|------------------------------|
| ['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis'] | ['Methanol', '67-56-1', 'PC-TWA', '25 mg/m <sup>3</sup> ', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.'] | ['', 'Remarks', 'Skin', 'None', 'None'] | ['', 'PC-STEL', '50 mg/m <sup>3</sup> ', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.'] | ['', 'Skin', 'None', 'None'] |
|--|---|---|---|------------------------------|

### Biological occupational exposure limits

|   |  |   |
|---|--|---|
| ['Component', 'CAS-No.', 'Parameters', 'Value', 'Biological specimen', 'Basis'] | ['Methanol', '67-56-1', 'Methanol', '15 mg/l', 'Urine', 'ACGIH - Biological Exposure Indices (BEI)'] | ['', 'Remarks', 'End of shift (As soon as possible after exposure ceases)', 'None', 'None', 'None'] |
|---|--|---|

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, 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 EC 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

Flame retardant antistatic protective clothing.

#### Respiratory protection

required when vapours/aerosols 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. Risk of explosion.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|  |                         |
|--|-------------------------|
| a) Physical state                          | liquid                  |
| b) Color                                   | white                   |
| c) Odor                                    | No data available       |
| d) Melting point/freezing point            | No data available       |
| e) Initial boiling point and boiling range | 64 - 65 °C at 1.013 hPa |
| f) Flammability (solid, gas)               | No data available       |

|   |  |
|---|--|
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 36 %(V)<br>Lower explosion limit: 6 %(V)                  |
| h) Flash point                                  | 9.7 °C - closed cup  |
| i) Autoignition temperature                     | No data available  |
| j) Decomposition temperature                    | No data available  |
| k) pH   | No data available  |
| l) Viscosity                                    | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                             | 8.3 g/L (20 °C)  |
| n) Partition coefficient n-octanol/water        | No data available  |
| o) Vapor pressure                               | No data available  |
| p) Density                                      | 0.791 g/cm <sup>3</sup> at 20 °C   |
| Relative density                                | 1.3640 (rough estimate)  |
| q) Relative vapor density                       | No data available  |
| r) Particle characteristics                     | No data available  |
| s) Explosive properties                         | Not classified as explosive.   |
| t) Oxidizing properties                         | none   |
| Solubility                                      | 0.1 M HCl: soluble   |

## 9.2 Other safety information

No data available

# SECTION 10: Stability and reactivity

## 10.1 Chemical stability

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

## 10.2 Possibility of hazardous reactions

No data available

## 10.3 Conditions to avoid

Warming.

## 10.4 Incompatible materials

Acids, Oxidizing agents, Alkali metals, Strong oxidizing agents, Strong acids, Acid chlorides,  
Acid anhydrides, Reducing agents, Strong reducing agents, Phosphorus halides

## 10.5 Hazardous decomposition products

In the event of fire: see section 5

# SECTION 11: Toxicological information

## 11.1 Information on toxicological effects

### Mixture Acute toxicity

Oral: No data available

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor (Calculation method)

Acute toxicity estimate Dermal - 300.4 mg/kg (Calculation method)

### Skin corrosion/irritation

Classified based on available data. For more details, see section 2

### Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

### Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

### Germ cell mutagenicity

Classified based on available data. For more details, see section 2

### Carcinogenicity

Classified based on available data. For more details, see section 2

### Reproductive toxicity

May harm the unborn child.

May impair fertility.

### Specific target organ toxicity - single exposure

Mixture causes damage to organs. - Eyes, Central nervous system

### Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

### Aspiration hazard

Classified based on available data. For more details, see section 2

## 11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Methyl alcohol may be fatal or cause blindness if swallowed., Cannot be made non- poisonous., Effects due to ingestion may include:, Nausea, Headache, Vomiting,

Gastrointestinal disturbance, Dizziness, Weakness, Confusion.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

### Components Methanol

#### Acute toxicity

Acute toxicity estimate Oral - 100.1 mg/kg (Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Symptoms: Nausea, Vomiting

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor (Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Symptoms: Irritation symptoms in the respiratory tract.

Acute toxicity estimate Dermal - 300.1 mg/kg (Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks: (ECHA)

Remarks: Drying-out effect resulting in rough and chapped skin.

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

Remarks: (ECHA)

#### **Respiratory or skin sensitization**

Sensitisation test: - Guinea pig

Result: negative (OECD Test Guideline 406)

#### **Germ cell mutagenicity**

Based on available data the classification criteria are not met.

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Bone marrow

Result: negative

#### **Carcinogenicity**

Did not show carcinogenic effects in animal experiments.

#### **Reproductive toxicity**

Based on available data the classification criteria are not met.

#### **Specific target organ toxicity - single exposure**

Causes damage to organs. - Eyes, Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Acute oral toxicity - Nausea, Vomiting

Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

#### **Specific target organ toxicity - repeated exposure**

Classified based on available data. For more details, see section 2

#### **Aspiration hazard**

Classified based on available data. For more details, see section 2

#### **Theophylline 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 (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

Result: negative

Remarks: (ECHA)

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Species: Mouse - male and female - Red blood cells (erythrocytes)

Result: negative

Remarks: (ECHA)

Species: Rat - male - sperm

Result: negative

Remarks: (ECHA)

Species: Mouse - male - Bone marrow

Result: negative

Remarks: (ECHA)

#### **Carcinogenicity**

Classified based on available data. For more details, see section 2

#### **Reproductive toxicity**

May damage the unborn child.

#### **Specific target organ toxicity - single exposure**

Classified based on available data. For more details, see section 2

#### **Specific target organ toxicity - repeated exposure Aspiration hazard**

Classified based on available data. For more details, see section 2

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## SECTION 12: Ecological information

### 12.1 Toxicity

#### **Mixture**

No data available

### 12.2 Persistence and degradability

No data available

### 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

#### Components Methanol

Toxicity to fish flow-through test LC50 - *Lepomis macrochirus* (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA)

Toxicity to daphnia semi-static test EC50 - *Daphnia magna* (Water flea) - 18,260 and other aquatic mg/l - 96 h invertebrates (OECD Test Guideline 202)

Toxicity to algae static test ErC50 - *Pseudokirchneriella subcapitata* (green algae) - ca. 22,000.0 mg/l - 96 h (OECD Test Guideline 201)

Toxicity to bacteria static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)

Toxicity to NOEC - *Oryzias latipes* (Orange-red killifish) - 7,900 mg/l - 200 fish(Chronic toxicity) h

Remarks: (External MSDS)

#### Theophylline

Toxicity to fish static test LC50 - *Leuciscus idus* (Golden orfe) - 100 mg/l - 96 h (DIN 38412 part 15)

Toxicity to daphnia static test EC50 - *Daphnia magna* (Water flea) - 178 mg/l - 48 and other aquatic h invertebrates (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)

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 1230

IMDG: 1230

IATA-DGR: 1230

## 14.2 UN proper shipping name

ADR/RID: METHANOL,SOLUTION

IMDG: METHANOL,SOLUTION

IATA-DGR: Methanol,SOLUTION

## 14.3 Transport hazard class(es)

ADR/RID: 3 (6.1)

IMDG: 3 (6.1)

IATA-DGR: 3 (6.1)

## 14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

## 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

## 14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

## 14.7 Incompatible materials

Acids, Oxidizing agents, Alkali metals, Strong oxidizing agents, Strong acids, Acid chlorides,

Acid anhydrides, Reducing agents, Strong reducing agents, Phosphorus halides

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# SECTION 15: Regulatory information

## 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

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# SECTION 16: Other information

## Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

**Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.