

**THEOPHYLLINE ANHYDROUS  
CAS NO 58-55-9**

**MATERIAL SAFETY DATA SHEET  
SDS/MSDS**

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

**1.1 Product identifiers**

Product name : Theophylline Anhydrous

CAS-No. : 58-55-9

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

Identified uses : Laboratory chemicals, Industrial & for professional use only.

**1.3 Details of the supplier of the safety data sheet**

Company : Central Drug House (P) Ltd  
7/28 Vardaan House  
New Delhi -110002  
INDIA

Telephone : +91 11 49404040  
Email : [care@cdhfinechemical.com](mailto:care@cdhfinechemical.com)

**1.4 Emergency telephone number**

Emergency Phone # : +91 11 49404040 (9:00am - 6:00 pm) [Office hours]

**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**

Hazard statement(s)  
H301 Toxic if swallowed.

Precautionary statement(s)  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.

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

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

#### Hazardous ingredients according to Regulation (EC) No 1272/2008

Component		Classification	Concentration
<b>Theophylline</b>			
CAS-No.	58-55-9	Acute Tox. 3; H301	<= 100 %
EC-No.	200-385-7		

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

Consult a physician. Show this safety data sheet to the doctor in attendance.

##### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

##### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

##### In case of eye contact

Flush eyes with water as a precaution.

##### If swallowed

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

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

No data available

### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

##### Suitable extinguishing media

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

### SECTION 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.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. 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

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

Store at Room Temperature.

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

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

### 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.

##### 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 (EN 143) respirator cartridges as a backup to engineering controls. If th 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.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |               |
|---------------|---------------|
| a) Appearance | Form: powder  |
|               | Colour: white |

b) Odour	odourless
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 274 - 275 °C
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) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	1.35 g/cm <sup>3</sup> at 25 °C
n) Water solubility	5.5 g/l at 19.9 °C
o) Partition coefficient: n-octanol/water	log Pow: -0.007 at 23 °C
p) Auto-ignition temperature	610 °C 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

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

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>) Other decomposition products - No data available

In the event of fire: see section 5

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - female - 272 mg/kg(Theophylline)  
LC50 Inhalation - Rat - male and female - 4 h - > 6.7  
mg/l(Theophylline) (OECD Test Guideline 403)  
LD50 Dermal - Rat - male and female - > 2,000  
mg/kg(Theophylline) (OECD Test Guideline 402)

#### Skin corrosion/irritation

Skin -  
Rabbit(Theophylline)  
Result: No skin irritation  
(OECD Test Guideline  
404)

#### Serious eye damage/eye irritation

Eyes -  
Rabbit(Theophylline)  
Result: No eye irritation  
(OECD Test Guideline  
405)

#### Respiratory or skin sensitisation

No data available(Theophylline)

#### Germ cell mutagenicity

Mouse(Theophylline)  
lymphocyte  
Result:  
negative  
(Theophylline)  
Mouse - male and female  
Result: negative

#### Carcinogenicity

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Theophylline)

#### Reproductive toxicity

No data available(Theophylline)

#### Specific target organ toxicity - single exposure

No data available(Theophylline)

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available(Theophylline)

#### Additional Information

RTECS: Not available  
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.(Theophylline)

## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish                      LC50 - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h(Theophylline)  
(DIN 38412)

Toxicity to daphnia and other aquatic invertebrates      static test EC50 - Daphnia magna (Water flea) - 178 mg/l - 48 h(Theophylline) (Directive 67/548/EEC, Annex V, C.2.)

Toxicity to algae      EC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h(Theophylline) (OECD Test Guideline 201)

#### 12.2 Persistence and degradability

Biodegradability      aerobic - Exposure time 22 d(Theophylline)  
Result: 90 - 100 % - Readily biodegradable

#### 12.3 Bioaccumulative potential

No data available

#### 12.4 Mobility in soil

No data available(Theophylline)

#### 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

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chem scrubber.

##### Contaminated packaging

Dispose of as unused product.

### 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 safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### 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.

### **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. Central Drug House (P) Ltd and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.cdhfinechemical.com](http://www.cdhfinechemical.com) for additional terms and conditions of sale.