



Preparing for the New Era of Laboratories

**SAFETY DATA SHEET**  
**(SDS)**

According to regulation (EU) no.1907/2006

**THEOPHYLLINE**  
**ANHYDROUS 99% Extrapure**

PRODUCT CODE : O-5290

CAS No : 58-55-9

FORMULA :  $C_7H_8N_4O_2$

UN No : 2811

# SAFETY DATA SHEET (SDS)

## THEOPHYLLINE ANHYDROUS 99% Extrapure



SDS Number : 0560

Date : May 6, 2026

Version : 1.0

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

- 1.1 Product Name** : THEOPHYLLINE ANHYDROUS 99% Extrapure  
**Synonyms** : 1,3-Dimethylxanthine,  
 3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione  
 2,6-Dihydroxy-1,3-dimethylpurine
- CAS No.** : 58-55-9  
**HS Code** : 2905 11 00  
**Chemical Formula** : C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>  
**Molecular Weight** : 180,16 g/mol  
**Product Code** : 0-5290  
**Brand** : Labotiq
- 1.2 Manufacturer** : Labotiq  
**Address** : Jl.Terapi Raya AD2-Bumi Menteng Asri Bogor, Jawa Barat Indonesia – 16111  
**Website** : [www.labotiq.net](http://www.labotiq.net)  
**Email** : [labotiq.id@gmail.com](mailto:labotiq.id@gmail.com)  
**For information** : Phone : (+62-251) 839110, 8311662, Fax : (+62-251) 83135710  
**Emergency number** : +6281316894650
- 1.3 Application** : Laboratory chemicals, Manufacture of substances, General Chemical reagent

### SECTION 2: Hazards identification

#### 2.1 Classification of the substance or mixture

##### Classification according to Regulation (EC) No 1272/2008

Acute toxicity, (Category 3) H301: Toxic if swallowed.  
 Reproductive toxicity, (Category 1B) H360D: May damage the unborn child.

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.

H360D

May damage the unborn child.

Precautionary statement(s)

P202

Do not handle until all safety precautions have been read and understood.

P264

Wash skin thoroughly after handling.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P301 + P310

IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

P405

Store locked up.

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P501 Dispose of contents/ container to an approved waste disposal plant.

Supplemental Hazard Statements none

Restricted to professional users

### 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.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 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<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

Index-No. : 613-342-00-6

### 3.2 Mixture

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

Component	Classification	Concentration
Theophylline No-CAS : 58-55-9 Nomor EC : 200-385-7 No-Indeks 613-342-00-6	Acute Tox. 3; Repr. 1B; H301, H360D	<=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 safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

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**In case of skin contact**

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

**In case of eye contact**

After eye contact: rinse out with plenty of water. Call in ophthalmologist. 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/vapours/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.

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**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****Advice on safe handling**

Work under hood. Do not inhale substance/mixture.

**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**

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

**Storage class**

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****8.2 Exposure controls****Appropriat 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**

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 EU Directive 89/686/EEC and the standard EN 374 derived from it.

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**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**

Appearance	Form: powder
	Colour: white
Odour	odourless
Odour Threshold	No data available
pH	No data available
Melting point/freezingpoint	Melting point/ range: 274 - 275 °C
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
Density	1,36 g/cm <sup>3</sup> at 25 °C
Relative density	No data available
Water solubility	5,5 g/l at 19,9 °C
Partition coefficient: noctanol/water	log Pow: -0,008 at 23 °C - Bioaccumulation is not expected.
Auto-ignition temperature	610 °C at 1.013 hPa
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

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**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).

**10.3 Possibility of hazardous reactions**

Violent reactions possible with: Strong oxidizing agents

**10.4 Conditions to avoid**

no information available.

**10.5 Incompatible materials**

No data available

**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)

Acute toxicity estimate Oral - 225 mg/kg

(ATE value derived from LD50/LC50 value)

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 sensitisation**

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

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Remarks: The value is given in analogy to the following substances: Caffeine

### Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Result: negative

Remarks: (ECHA)

Test Type: Chromosome aberration test

Species: Rat

Cell type: sperm

Application Route: Oral

Result: negative

Remarks: (ECHA)

Test Type: Chromosome aberration test

Species: Mouse

Cell type: Bone marrow

Application Route: Intraperitoneal

Result: negative

Remarks: (ECHA)

### Carcinogenicity

No data available

### Reproductive toxicity

May damage the unborn child.

### Specific target organ toxicity - single exposure

No data available

### Specific target organ toxicity - repeated exposure

No data available

### Aspiration hazard

No aspiration toxicity classification

### Additional Information

Endocrine disrupting properties

Product:

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**Assessment :**

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher. Repeated dose toxicity - Rat - male and female - Oral - 13 Weeks - Lowest observed adverse effect level - 37,5 mg/kg

Remarks: (ECHA)

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.

### SECTION 12: Ecological information

#### 12.1 Toxicity

Toxicity to fish

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

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

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)

#### 12.2 Persistence and degradability

Biodegradability

aerobic - Exposure time 22 d

Result: > 90 - 100 % -

Readily biodegradable. (OECD Test Guideline 301A)

#### 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

Endocrine disrupting properties

Product:

Assessment :

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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### SECTION 13: Disposal considerations

#### 13.1 Waste treatment methods

No data available

### 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

#### 14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

### 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.

##### Authorisations and/or restrictions on use

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII) : Theophylline

##### National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

H2 ACUTE TOXIC

#### 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.

H360D May damage the unborn child.

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**National Fire Protection Association (U.S.A.):**

Health: 3

Flammability: 1

Reactivity: 0

**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. Labotiq shall not be held liable for any damage resulting from handling or from contact with the above product.*

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