

According to Regulation (EC) No. 1907/2006

Creation Date: May 17, 2026

Revision Date: May 17, 2026

1. IDENTIFICATION

1.1 GHS Product identifier

Product name: Theophylline

Catalog Number: T1083

CAS Number: 58-55-9

1.2 Other means of identification

Other names: -

1.3 Recommended use of the chemical and restrictions on use

Identified uses: no data available

1.4 Supplier's details

Company: Targetmol Chemicals Inc.

Address: 34 Washington Street, Wellesley Hills, Massachusetts 02481 USA

Tel/Fax: (781) 999-4286

1.5 Emergency phone number

Emergency phone number: 781-999-4286

Service hours: Monday to Friday, 9am-5pm (Standard timezone: UTC/GMT -5 hours).

2. HAZARD IDENTIFICATION

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Acute toxicity - Category 3, Oral

2.2 GHS label elements, including precautionary statements

Labelling according to Regulation (EC) No 1272/2008

The substance is classified and labelled according to the CLP regulation.

Pictogram(s): unknown

Signal word: Danger

Hazard statement(s): H301 Toxic if swallowed

Precautionary statement(s):

Prevention: P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.

Response: P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.

Storage: P405 Store locked up.

Disposal: P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number
Theophylline	-	58-55-9	200-385-7

4. FIRST-AID MEASURES

4.1 Description of necessary first-aid measures

General advice

no data available

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

Following eye contact

Rinse with plenty of water for several minutes (remove contact lenses if easily possible).

Following ingestion

Rinse mouth. Give a slurry of activated charcoal in water to drink. Refer for medical attention.

4.2 Most important symptoms/effects, acute and delayed

no data available

4.3 Indication of immediate medical attention and special treatment needed, if necessary

no data available

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

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

5.2 Specific hazards arising from the chemical

Not combustible. Gives off irritating or toxic fumes (or gases) in a fire.

5.3 Special protective actions for fire-fighters

In case of fire in the surroundings, use appropriate extinguishing media.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into sealable containers. If appropriate, moisten first to prevent dusting. Then store and dispose of according to local regulations.

6.2 Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with

appropriate laws and regulations.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs.

Powder: -20°C for 3 years | In solvent: -80°C for 1 year

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Avoid inhalation of dust and mist.

Thermal hazards

no data available

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state	Solid
Color	White
Odour	no data available
Melting point/freezing point	270 - 274 °C.
Boiling point or initial boiling point and boiling range	384°C(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	88°C(lit.)
Auto-ignition temperature	610 °C. Atm. press.:1 013 hPa.
Decomposition temperature	no data available
pH	no data available

Kinematic viscosity	no data available
Solubility	DMSO: 16.83 mg/mL (93.42 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
N-octanol-water partition coefficient	log Pow = -0.008. Temperature:23 °C.
Vapour pressure	0.001 mBar. Temperature:20 °C.
Density and/or relative density	1.36 g/cm ³ . Temperature:25 °C.
Relative vapour density	no data available
Particle characteristics	no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

Decomposes on heating. This produces toxic fumes including nitrogen oxides.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Oral: LD50 - rat (female) - 272 mg/kg bw.

Inhalation: LC50 - rat (male/female) - > 6.7 mg/L air.

Dermal: LD50 - rat (male/female) - > 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance may cause effects on the heart and central nervous system. This may result in cardiac dysrhythmia and convulsions. The effects may be delayed.

STOT-repeated exposure

no data available

Aspiration hazard

A nuisance-causing concentration of airborne particles can be reached quickly when dispersed.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish: LC50 - *Leuciscus idus* - 100 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 178 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - > 100 mg/L - 72 h.

Toxicity to microorganisms: EC80 - activated sludge - > 1 000 mg/L - 180 min.

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 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

14. TRANSPORT INFORMATION

14.1 UN Number

no data available

14.2 UN Proper Shipping Name

no data available

14.3 Transport hazard class(es)

no data available

14.4 Packing group, if applicable

no data available

14.5 Environmental hazards

no data available

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations specific for the product in question

This safety data sheet complies with the requirements of Regulation (EC) No.1907/2006.

European Inventory of Existing Commercial Chemical Substances (EINECS)	Listed.
EC Inventory	Listed.
United States Toxic Substances Control Act (TSCA) Inventory	Listed.
China Catalog of Hazardous chemicals 2015	Not Listed.
New Zealand Inventory of Chemicals (NZIPC)	Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Listed.
Vietnam National Chemical Inventory	Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Listed.
Korea Existing Chemicals List (KECL)	Listed.

16. OTHER INFORMATION

Information on revision

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Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_l°Cale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Other Information

no data available

Disclaimer: 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. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product. All products are for Research Use Only · Not For Human or Veterinary or Therapeutic Use