1 Identification

Product identifier
Product name: Theophylline monohydrate
Stock number: A15997
CAS Number: 5967-84-0
EC number: 200-385-7

Relevant identified uses of the substance or mixture and uses advised against.
Identified use: SU24   Scientific research and development

Details of the supplier of the safety data sheet
Manufacturer/Supplier:
Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-543-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:
During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)
GHS06 Skull and crossbones
Acute Tox. 3 H301 Toxic if swallowed.

Hazard(s) not otherwise classified No information known.

Label elements
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms

GHS06

Signal word Danger

Hazard statements
H301 Toxic if swallowed.

Precautionary statements
P264 Wash thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...
P321 Specific treatment (see on this label).
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification
D1B - Toxic material causing immediate and serious toxic effects

Classification system
HMIS ratings (scale 0-4)
(Hazardous Materials Identification System)

 Health (acute effects) = 2
 Flammability = 1
 Physical Hazard = 1

Other hazards
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances
CAS# Description: 5967-84-0 Theophylline monohydrate
Identification number(s):
EC number: 200-385-7

4 First-aid measures

Description of first aid measures
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm. Seek immediate medical advice.

After skin contact
Immediately wash with water and soap and rinse thoroughly. Seek immediate medical advice.

After eye contact
Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing
Seek medical treatment.
5 Fire-fighting measures

Extinguishing media

- Suitable extinguishing agents: Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

- If this product is involved in a fire, the following can be released:
  - Carbon monoxide and carbon dioxide
  - Nitrogen oxides (NOx)

Advice for firefighters

- Protective equipment:
  - Wear self-contained respirator.
  - Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

- Wear protective equipment. Keep unprotected persons away.

Environmental precautions:

- Do not allow material to be released to the environment without proper governmental permits.

Methods and material for containment and cleaning up:

- Dispose of contaminated material as waste according to section 13.

Prevention of secondary hazards:

- No special measures required.

Reference to other sections

- See Section 7 for information on safe handling
- See Section 8 for information on personal protection equipment
- See Section 13 for disposal information

7 Handling and storage

Handling

- Precautions for safe handling:
  - Keep container tightly sealed.
  - Store in cool, dry place in tightly closed containers.
  - Ensure good ventilation at the workplace.

Information about protection against explosions and fires:

- No information known.

Storage

- Requirements to be met by storerooms and receptacles:
  - No special requirements.

Information about storage in one common storage facility:

- Store away from oxidizing agents.

Further information about storage conditions:

- Keep container tightly sealed.
- Store in cool, dry conditions in well sealed containers.

Specific end use(s):

- No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:

- Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:

- The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.

Additional information:

- No data

Exposure controls

Personal protective equipment

- General protective and hygienic measures:
  - The usual precautionary measures for handling chemicals should be followed.
  - Keep away from foodstuffs, beverages and feed.
  - Remove all soiled and contaminated clothing immediately.
  - Wash hands before breaks and at the end of work.
  - Maintain an ergonomically appropriate working environment.

- Breathing equipment:
  - Use suitable respirator when high concentrations are present.
  - Recommended filter device for short term use:
    - Use a respirator with type P100 (USA) or P3 (EN 143) cartridges as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards.

Protection of hands:

- Impervious gloves
  - Check protective gloves prior to each use for their proper condition.
  - The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

- Penetration time of glove material (in minutes):
  - Not determined

Eye protection:

- Safety glasses

Body protection:

- Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General information

- Appearance:
  - Powder
  - White
  - Odorless
  - Odor threshold:
    - Not determined.

- pH-value:
  - Not applicable.

Change in condition

- Melting point/Melting range:
  - 270-274 °C (518-525 °F)
- Boiling point/Boiling range:
  - Not determined
- Sublimation temperature / start:
  - Not determined
- Flash point:
  - Not applicable
- Flash point:
  - Not determined
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined

Danger of explosion: Product does not present an explosion hazard.

Explosion limits:
- Lower: Not determined
- Upper: Not determined

Vapor pressure: Not applicable.

Relative density: Not determined.

Vapor density: Not applicable.

Evaporation rate: Not applicable.

Solubility in / Miscibility with Water at 20 °C (68 °F): 8 g/l

Partition coefficient (n-octanol/water): Not determined.

Viscosity:
- Dynamic: Not applicable.
- Kinematic: Not applicable.

Other information: No further relevant information available.

10 Stability and reactivity

Reactivity: No information known.
Chemical stability: Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.
Possibility of hazardous reactions: Reacts with strong oxidizing agents.
Conditions to avoid: No further relevant information available.
Incompatible materials: Oxidizing agents.
Hazardous decomposition products: Carbon monoxide and carbon dioxide, Nitrogen oxides.

11 Toxicological information

Information on toxicological effects

Acute toxicity:
- Toxic if swallowed.

The following RTECS statement/statements refer to the anhydrous compound:
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for this substance.

LD/LC50 values that are relevant for classification:
The following values/references refer to the anhydrous compound:

<table>
<thead>
<tr>
<th>Route</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral</td>
<td>183 mg/kg (guinea pig)</td>
</tr>
<tr>
<td></td>
<td>235 mg/kg (mouse)</td>
</tr>
<tr>
<td></td>
<td>225 mg/kg (rat)</td>
</tr>
<tr>
<td></td>
<td>350 mg/kg (rabbit)</td>
</tr>
</tbody>
</table>

Skin irritation or corrosion: May cause irritation
Eye irritation or corrosion: May cause irritation
Sensitization: No sensitizing effects known.
Germ cell mutagenicity: The following RTECS statement/statements refer to the anhydrous compound:
The Registry of Toxic Effects of Chemical Substances (RTECS) contains mutation data for this substance.
Carcinogenicity: IARC-3: Not classifiable as to carcinogenicity to humans.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: No effects known.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: The following RTECS statement/statements refer to the anhydrous compound:
The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for this substance.

Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity: No further relevant information available.
Aquatic toxicity: No further relevant information available.
Persistence and degradability: No further relevant information available.
Bioaccumulative potential: No further relevant information available.
Mobility in soil: No further relevant information available.

General notes:
Do not allow material to be released to the environment without proper governmental permits.
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.

13 Disposal considerations

Waste treatment methods
Recommendation: Consult state, local or national regulations to ensure proper disposal.

Uncleaned packaging:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number: UN2811
DOT, IMDG, IATA: USA
### Transport hazard class(es)

**DOT**

<table>
<thead>
<tr>
<th>Class</th>
<th>Label</th>
</tr>
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<tbody>
<tr>
<td>6.1</td>
<td>Toxic substances.</td>
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**IMDG, IATA**

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<td>Toxic substances.</td>
</tr>
</tbody>
</table>

### Packing group

**DOT, IMDG, IATA**

- III

### Environmental hazards:

- Not applicable.

### Special precautions for user

**EMS Number:** Warning: Toxic substances

**Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**

- Not applicable.

### Transport/Additional information:

**DOT**

- Marine Pollutant (DOT): No

**UN "Model Regulation":** UN2811, Toxic solids, organic, n.o.s. (Theophylline monohydrate), 6.1, III

### 15 Regulatory information

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

**GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

**Hazard pictograms**

- GHS06

**Signal word** Danger

**Hazard statements**

- H301 Toxic if swallowed.

**Precautionary statements**

- P264 Wash thoroughly after handling.
- P270 Do not eat, drink or smoke when using this product.
- P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/…
- P321 Specific treatment (see on this label).
- P405 Store locked up.
- P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

**National regulations**

All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.

All components of this product are listed on the Canadian Domestic Substances List (DSL).

**SARA Section 313 (specific toxic chemical listings)** Substance is not listed.

**California Proposition 65**

- Prop 65 - Chemicals known to cause cancer Substance is not listed.
- Prop 65 - Developmental toxicity Substance is not listed.
- Prop 65 - Developmental toxicity, male Substance is not listed.
- Prop 65 - Developmental toxicity, female Substance is not listed.

**Prop 65 - Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006** Substance is not listed.

The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.

**Substance is not listed.**

**Annex XIV of the REACH Regulations (requiring Authorisation for use)** Substance is not listed.

**Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

### 16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper control and protection of the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

**Department issuing SDS:** Global Marketing Department

**Date of preparation / last revision** 11/23/2015

**Abbreviations and acronyms:**

- RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
- IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)
- ICAO: International Civil Aviation Organization
- ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)
- ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
- IMDG: International Maritime Code for Dangerous Goods
- DOT: US Department of Transportation
- IATA: International Air Transport Association
- EINECS: European Inventory of Existing Commercial Chemical Substances
- CAS: Chemical Abstracts Service (division of the American Chemical Society)
- HMIS: Hazardous Materials Identification System (USA)
- WHMIS: Workplace Hazardous Materials Information System (Canada)
- LC50: Lethal concentration, 50 percent
- LD50: Lethal dose, 50 percent
- vPvB: very Persistent and very Bioaccumulative
Product name: Theophylline monohydrate

ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)