1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name: 7-(β-Hydroxyethyl)theophylline
Product Number: H9006
Brand: Sigma
CAS-No.: 519-37-9

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

Identified uses: Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone: +1 800-325-5832
Fax: +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone #: (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Acute toxicity, Oral (Category 4), H302

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word: Warning
Hazard statement(s)
H302 Harmful if swallowed.
Precautionary statement(s)
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P301 + P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
P330 Rinse mouth.
P501 Dispose of contents/container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms: 1,3-Dimethyl-7-(2-hydroxyethyl)xanthine
**Formula**: C₉H₁₂N₄O₃
**Molecular Weight**: 224.22 g/mol
**CAS-No.**: 519-37-9
**EC-No.**: 208-269-8

**Hazardous components**

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Etofylline</td>
<td>Acute Tox. 4; H302</td>
<td>-</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 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. Move out of dangerous area.

**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. 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

### 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 (NOx)

#### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

#### 5.4 Further information

No data available

### 6. ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

For personal protection see section 8.

#### 6.2 Environmental precautions

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.

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. Normal measures for preventive fire protection. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters
Components with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Safety glasses with side-shields conforming to EN166 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
For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance
Form: solid

b) Odour
no data available

c) Odour Threshold
no data available

d) pH
no data available

e) Melting point/freezing point
no data available

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 no data available
n) Water solubility no data available
o) Partition coefficient: n-octanol/water no data available
p) Auto-ignition temperature no data available
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

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
no data available

10.6 Hazardous decomposition products
Other decomposition products - no data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - rat - 710 mg/kg
Remarks: Liver:Other changes.
Inhalation: no data available
Dermal: no data available
Skin corrosion/irritation
no data available
**Serious eye damage/eye irritation**  
no data available

**Respiratory or skin sensitisation**  
no data available

**Germ cell mutagenicity**  
no data available

**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**  
no data available

Reproductive toxicity - rat - Oral  
Maternal Effects: Uterus, cervix, vagina.

no data available

**Specific target organ toxicity - single exposure**  
no data available

**Specific target organ toxicity - repeated exposure**  
no data available

**Aspiration hazard**  
no data available

**Additional Information**

RTECS: XH5850000

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

---

**12. ECOLOGICAL INFORMATION**

**12.1 Toxicity**  
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 Other adverse effects**  
no data available
13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

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

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Etofylline</td>
<td>519-37-9</td>
<td></td>
</tr>
</tbody>
</table>

New Jersey Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Etofylline</td>
<td>519-37-9</td>
<td></td>
</tr>
</tbody>
</table>

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.  Acute toxicity
H302  Harmful if swallowed.

HMIS Rating
Health hazard: 1
Chronic Health Hazard: 0
Flammability: 0
Physical Hazard: 0

NFPA Rating
Health hazard: 1
Fire Hazard: 0
Reactivity Hazard: 0

Further information
Copyright 2014 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. 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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 4.2  Revision Date: 07/01/2014  Print Date: 06/21/2016