

**SAFETY DATA SHEET**

Creation Date 21-May-2015

Revision Date 26-Mar-2024

Revision Number 4

**1. Identification**

**Product Name** Theophylline-7-acetic acid

**Cat No. :** L06812

**CAS No** 652-37-9  
**Synonyms** 1,3-Dimethylxanthine-7-acetic acid; Acefylline

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

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

Thermo Fisher Scientific Chemicals, Inc.  
30 Bond Street  
Ward Hill, MA 01835-8099  
Tel: 800-343-0660  
Fax: 800-322-4757

**Emergency Telephone Number**

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
**Emergency Number US:**001-201-796-7100 / **Europe:** +32 14 57 52 99  
**CHEMTREC** Tel. No. **US:**001-800-424-9300 / **Europe:**001-703-527-3887

**2. Hazard(s) identification****Classification**

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

|  |            |
|--|------------|
| Acute oral toxicity                              | Category 4 |
| Skin Corrosion/Irritation                        | Category 2 |
| Serious Eye Damage/Eye Irritation                | Category 2 |
| Specific target organ toxicity (single exposure) | Category 3 |
| Target Organs - Respiratory system.              |            |

**Label Elements****Signal Word**

Warning

**Hazard Statements**

Harmful if swallowed

Causes skin irritation  
Causes serious eye irritation  
May cause respiratory irritation

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling  
Do not eat, drink or smoke when using this product  
Wear protective gloves/protective clothing/eye protection/face protection  
Avoid breathing dust/fume/gas/mist/vapors/spray  
Use only outdoors or in a well-ventilated area

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
Call a POISON CENTER or doctor/physician if you feel unwell

**Skin**

IF ON SKIN: Wash with plenty of soap and water  
If skin irritation occurs: Get medical advice/attention  
Take off contaminated clothing and wash before reuse

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
If eye irritation persists: Get medical advice/attention

**Ingestion**

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
Rinse mouth

**Storage**

Store in a well-ventilated place. Keep container tightly closed  
Store locked up

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

None identified

### 3. Composition/Information on Ingredients

| Component                   | CAS No   | Weight % |
|-----------------------------|----------|----------|
| Theophyllin-7-ylacetic acid | 652-37-9 | >95      |

### 4. First-aid measures

**General Advice**

If symptoms persist, call a physician.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

|  |   |
|--|---|
| <b>Ingestion</b>                           | Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur. |
| <b>Most important symptoms and effects</b> | None reasonably foreseeable.  |
| <b>Notes to Physician</b>                  | Treat symptomatically   |

## 5. Fire-fighting measures

|   |   |
|---|---|
| <b>Suitable Extinguishing Media</b>     | Water spray, carbon dioxide (CO <sub>2</sub> ), dry chemical, alcohol-resistant foam. |
| <b>Unsuitable Extinguishing Media</b>   | No information available  |
| <b>Flash Point</b>                      | Not applicable  |
| <b>Method -</b>                         | No information available  |
| <b>Autoignition Temperature</b>         | No information available  |
| <b>Explosion Limits</b>                 |   |
| <b>Upper</b>                            | No data available   |
| <b>Lower</b>                            | No data available   |
| <b>Sensitivity to Mechanical Impact</b> | No information available  |
| <b>Sensitivity to Static Discharge</b>  | No information available  |

### Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

### Hazardous Combustion Products

Carbon monoxide (CO). Nitrogen oxides (NO<sub>x</sub>). Carbon dioxide (CO<sub>2</sub>).

### Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

### NFPA

**Health**  
2

**Flammability**  
1

**Instability**  
1

**Physical hazards**  
N/A

## 6. Accidental release measures

|   |  |
|---|--|
| <b>Personal Precautions</b>                 | Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.            |
| <b>Environmental Precautions</b>            | Should not be released into the environment. See Section 12 for additional Ecological Information.           |
| <b>Methods for Containment and Clean Up</b> | Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal. |

## 7. Handling and storage

|                 |   |
|-----------------|---|
| <b>Handling</b> | Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation. |
| <b>Storage.</b> | Keep containers tightly closed in a dry, cool and well-ventilated place. Protect from moisture. Store under an inert atmosphere. Incompatible Materials. Strong oxidizing agents.   |

## 8. Exposure controls / personal protection

|                            |   |
|----------------------------|---|
| <b>Exposure Guidelines</b> | This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies. |
|----------------------------|---|

**Engineering Measures** Ensure that eyewash stations and safety showers are close to the workstation location.

**Personal Protective Equipment**

**Eye/face Protection** Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure.

**Respiratory Protection** Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

**Recommended Filter type:** Particulates filter conforming to EN 143.

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

|  |                          |
|--|--------------------------|
| Physical State                         | Solid                    |
| Appearance                             | No information available |
| Odor                                   | No information available |
| Odor Threshold                         | No information available |
| pH                                     | Not applicable           |
| Melting Point/Range                    | 270 °C / 518 °F          |
| Boiling Point/Range                    | Not applicable           |
| Flash Point                            | Not applicable           |
| Evaporation Rate                       | Not applicable           |
| Flammability (solid,gas)               | No information available |
| Flammability or explosive limits       |                          |
| Upper                                  | No data available        |
| Lower                                  | No data available        |
| Vapor Pressure                         | No information available |
| Vapor Density                          | Not applicable           |
| Specific Gravity                       | No information available |
| Solubility                             | No information available |
| Partition coefficient; n-octanol/water | No data available        |
| Autoignition Temperature               | No information available |
| Decomposition Temperature              | No information available |
| Viscosity                              | Not applicable           |
| Molecular Formula                      | C9 H10 N4 O4             |
| Molecular Weight                       | 238.2                    |

## 10. Stability and reactivity

|                                  |   |
|----------------------------------|---|
| Reactive Hazard                  | None known, based on information available  |
| Stability                        | Hygroscopic.  |
| Conditions to Avoid              | Incompatible products. Excess heat. Avoid dust formation. Exposure to moist air or water. |
| Incompatible Materials           | Strong oxidizing agents   |
| Hazardous Decomposition Products | Carbon monoxide (CO), Nitrogen oxides (NOx), Carbon dioxide (CO <sub>2</sub> )            |
| Hazardous Polymerization         | Hazardous polymerization does not occur.  |

**Hazardous Reactions** None under normal processing.

## 11. Toxicological information

### Acute Toxicity

#### Product Information

#### Component Information

| Component                   | LD50 Oral                | LD50 Dermal | LC50 Inhalation |
|-----------------------------|--------------------------|-------------|-----------------|
| Theophyllin-7-ylacetic acid | LD50 = 900 mg/kg ( Rat ) | Not listed  | Not listed      |

**Toxicologically Synergistic** No information available

#### Products

#### Delayed and immediate effects as well as chronic effects from short and long-term exposure

**Irritation** No information available

**Sensitization** No information available

**Carcinogenicity** The table below indicates whether each agency has listed any ingredient as a carcinogen.

| Component                   | CAS No   | IARC       | NTP        | ACGIH      | OSHA       | Mexico     |
|-----------------------------|----------|------------|------------|------------|------------|------------|
| Theophyllin-7-ylacetic acid | 652-37-9 | Not listed | Not listed | Not listed | Not listed | Not listed |

**Mutagenic Effects** No information available

**Reproductive Effects** No information available.

**Developmental Effects** No information available.

**Teratogenicity** No information available.

**STOT - single exposure** Respiratory system

**STOT - repeated exposure** None known

**Aspiration hazard** No information available

**Symptoms / effects, both acute and delayed** No information available

**Endocrine Disruptor Information** No information available

**Other Adverse Effects** The toxicological properties have not been fully investigated.

## 12. Ecological information

### Ecotoxicity

Do not empty into drains.

**Persistence and Degradability** No information available

**Bioaccumulation/ Accumulation** No information available.

**Mobility** No information available.

## 13. Disposal considerations

#### Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## 14. Transport information

|                 |               |
|-----------------|---------------|
| <b>DOT</b>      | Not regulated |
| <b>TDG</b>      | Not regulated |
| <b>IATA</b>     | Not regulated |
| <b>IMDG/IMO</b> | Not regulated |

## 15. Regulatory information

### United States of America Inventory

| Component                   | CAS No   | TSCA | TSCA Inventory notification -<br>Active-Inactive | TSCA - EPA Regulatory<br>Flags |
|-----------------------------|----------|------|--|--------------------------------|
| Theophyllin-7-ylacetic acid | 652-37-9 | -    | -  | -                              |

#### **Legend:**

**TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)** Not applicable

**TSCA 12(b)** - Notices of Export Not applicable

### International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

| Component                   | CAS No   | DSL | NDSL | EINECS    | PICCS | ENCS | ISHL | AICS | IECSC | KECL |
|-----------------------------|----------|-----|------|-----------|-------|------|------|------|-------|------|
| Theophyllin-7-ylacetic acid | 652-37-9 | -   | -    | 211-490-2 | -     | -    |      | -    | -     | -    |

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

### U.S. Federal Regulations

#### **SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

#### **SARA 311/312 Hazard Categories**

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

**CWA (Clean Water Act)** Not applicable

**Clean Air Act** Not applicable

**OSHA** - Occupational Safety and Health Administration Not applicable

#### **CERCLA**

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

**California Proposition 65** This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations** Not applicable

**U.S. Department of Transportation**

Reportable Quantity (RQ): N  
DOT Marine Pollutant N  
DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** No information available

**Authorisation/Restrictions according to EU REACH** Not applicable

| Component                   | CAS No   | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|-----------------------------|----------|---|---|---|
| Theophyllin-7-ylacetic acid | 652-37-9 | -   | -   | -   |

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

| Component                   | CAS No   | OECD HPV       | Persistent Organic Pollutant | Ozone Depletion Potential | Restriction of Hazardous Substances (RoHS) |
|-----------------------------|----------|----------------|------------------------------|---------------------------|--|
| Theophyllin-7-ylacetic acid | 652-37-9 | Not applicable | Not applicable               | Not applicable            | Not applicable                             |

**Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?**

Not applicable

**Other International Regulations**

| Component                   | CAS No   | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements | Rotterdam Convention (PIC) | Basel Convention (Hazardous Waste) |
|-----------------------------|----------|---|--|----------------------------|------------------------------------|
| Theophyllin-7-ylacetic acid | 652-37-9 | Not applicable  | Not applicable   | Not applicable             | Not applicable                     |

**16. Other information**

**Prepared By** Health, Safety and Environmental Department  
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**Creation Date** 21-May-2015  
**Revision Date** 26-Mar-2024  
**Print Date** 26-Mar-2024  
**Revision Summary** New emergency telephone response service provider.

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of SDS**