

SAFETY DATA SHEET

Creation Date 21-May-2015

Revision Date 26-March-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****Importer/Distributor**

Fisher Scientific
112 Colonnade Road,
Ottawa, ON K2E 7L6,
Canada
Tel: 1-800-234-7437

Emergency Telephone NumberFor information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11Emergency 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****WHMIS 2015 Classification**

Classified as hazardous under the Hazardous Products Regulations (SOR/2015-17)

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**

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

Response

IF ON SKIN: Wash with plenty of soap and water
IF INHALED: Remove person to fresh air and keep comfortable for breathing
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
Call a POISON CENTER/ doctor if you feel unwell
Rinse mouth
Take off contaminated clothing and wash it before reuse

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

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

5. Fire-fighting measures

Suitable Extinguishing Media Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam.

Unsuitable Extinguishing Media No information available

Flash Point Not applicable
Method - No information available

Autoignition Temperature No information available

Explosion Limits

Upper No data available

Lower No data available

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge 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_x). Carbon dioxide (CO₂).

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

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

Environmental Precautions Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

7. Handling and storage

Handling 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.

Storage. 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

Exposure Guidelines 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. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection
Hand ProtectionGoggles
Wear appropriate protective gloves and clothing to prevent skin exposure.

Glove material	Breakthrough time	Glove thickness	Glove comments
Nitrile rubber Neoprene Natural rubber PVC	See manufacturers recommendations	-	Splash protection only

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. 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. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Recommended Filter type: Particulates filter conforming to EN 143

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls

No information available.

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 ₂)
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 Products No information available

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

DOT Not regulated
TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory information

International Inventories

Component	CAS-No	DSL	NDSL	TSCA	TSCA Inventory notification - Active-Inactive	EINECS	ELINCS	NLP
Theophyllin-7-ylacetic acid	652-37-9	-	-	-	-	211-490-2	-	-

Component	CAS-No	IECSC	KECL	ENCS	ISHL	TCSI	AICS	NZIoC	PICCS
Theophyllin-7-ylacetic acid	652-37-9	-	-	-	-	X	-	-	-

Legend:

X - Listed '-' - Not Listed

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

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

Canada

SDS in compliance with provisions of information as set out in Canadian Standard - Part 4, Schedule 1 and 2 of the Hazardous Products Regulations (HPR) and meets the requirements of the HPR (Paragraph 13(1)(a) of the Hazardous Products Act (HPA)).

Other International Regulations

Authorisation/Restrictions according to EU REACH Not applicable

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

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	Product Safety Department Email: chem.techinfo@thermofisher.com www.thermofisher.com
Creation Date	21-May-2015
Revision Date	26-March-2024
Print Date	26-March-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