

ALFAAL04570

## 8-Chlorotheophylline

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

<b>产品说明:</b> <b>Product Description:</b>	<b>8-Chlorotheophylline</b> <b>8-Chlorotheophylline</b>
<b>Cat No. :</b>	<b>L04570</b>
<b>Synonyms</b>	8-Chloro-1,3-dimethyl-2,6(1H,3H)-purinedione
<b>CAS No</b>	85-18-7
<b>Molecular Formula</b>	C7 H7 Cl N4 O2
<b>Supplier</b>	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
<b>Emergency Telephone Number</b>	For information <b>US</b> call: 001-800-227-6701 / <b>Europe</b> call: +32 14 57 52 11 Emergency Number <b>US</b> :001-201-796-7100 / <b>Europe</b> : +32 14 57 52 99 <b>CHEMTREC</b> Tel. No. <b>US</b> :001-800-424-9300 / <b>Europe</b> :001-703-527-3887
<b>E-mail address</b>	begel.sdsdesk@thermofisher.com
<b>Recommended Use</b> <b>Uses advised against</b>	Laboratory chemicals. No Information available

### SECTION 2. HAZARD IDENTIFICATION

<b>Physical State</b> Powder Solid	<b>Appearance</b> White	<b>Odor</b> Odorless
<b>Emergency Overview</b> Harmful if swallowed. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation. May form combustible dust concentrations in air.		

#### Classification of the substance or mixture

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

#### Label Elements



## 8-Chlorotheophylline

## Signal Word

## Warning

## Hazard Statements

H302 - Harmful if swallowed  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

## Precautionary Statements

## Prevention

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P270 - Do not eat, drink or smoke when using this product  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

## Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P330 - Rinse mouth  
P362 + P364 - Take off contaminated clothing and wash it before reuse

## Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

## Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

## Physical and Chemical Hazards

None identified. May form combustible dust concentrations in air.

## Health Hazards

Harmful if swallowed. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

## Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

May form explosible dust-air mixture if dispersed. This product does not contain any known or suspected endocrine disruptors.

## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
8-Chlorotheophylline	85-18-7	99

## SECTION 4. FIRST AID MEASURES

## 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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.

## Inhalation

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

## Ingestion

Clean mouth with water. Get medical attention.

## Most important symptoms and effects

No information available.

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Fine dust dispersed in air may ignite.

**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.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation.

**Environmental Precautions**

See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Avoid dust formation. Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Avoid contact with skin and eyes. Do not breathe dust. Do not ingest. If swallowed then seek immediate medical assistance.

**Storage**

Keep in a dry, cool and well-ventilated place. Keep container tightly closed.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

## 8-Chlorotheophylline

## Exposure Controls

## Engineering Measures

Ensure adequate ventilation, especially in confined areas. 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** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, 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.

Remove gloves with care avoiding skin contamination.

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

**Respiratory Protection** No protective equipment is needed under normal use conditions.

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

**Small scale/Laboratory use** Maintain adequate ventilation

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

**Environmental exposure controls** No information available.

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance</b>	White	
<b>Physical State</b>	Powder Solid	
<b>Odor</b>	Odorless	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	290 °C / 554 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flash Point</b>	No information available	<b>Method -</b> No information available Solid
<b>Evaporation Rate</b>	Not applicable	
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Specific Gravity / Density</b>	No data available	

## 8-Chlorotheophylline

Bulk Density	No data available	
Water Solubility	slightly soluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	Not applicable	Solid
Explosive Properties	No information available	
Oxidizing Properties	No information available	

Molecular Formula	C7 H7 Cl N4 O2
Molecular Weight	214.61

## SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	No information available.
Hazardous Polymerization	No information available.
Conditions to Avoid	Incompatible products.
Materials to avoid	Strong oxidizing agents. Oxidizing agent.

**Hazardous Decomposition Products** Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

(a) acute toxicity;	
(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization;	
Respiratory	No data available
Skin	No data available
(e) germ cell mutagenicity;	No data available
(f) carcinogenicity;	No data available
	There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	Category 3
Results / Target organs	Respiratory system
(i) STOT-repeated exposure;	No data available

**Target Organs**

No information available.

**(j) aspiration hazard;**Not applicable  
Solid**Other Adverse Effects**

The toxicological properties have not been fully investigated.

**Symptoms / effects, both acute and delayed** No information available**SECTION 12. ECOLOGICAL INFORMATION****Ecotoxicity effects**

Do not empty into drains.

**Persistence and Degradability  
Persistence**

Soluble in water, Persistence is unlikely, based on information available.

**Bioaccumulative Potential**

Bioaccumulation is unlikely

**Mobility in soil**

The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility Highly mobile in soils

**Endocrine Disruptor Information  
Persistent Organic Pollutant  
Ozone Depletion Potential**This product does not contain any known or suspected endocrine disruptors  
This product does not contain any known or suspected substance  
This product does not contain any known or suspected substance**SECTION 13. DISPOSAL CONSIDERATIONS****Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point.

**Other Information**

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

**SECTION 14. TRANSPORT INFORMATION****Road and Rail Transport**

Not Regulated

**IMDG/IMO**

Not regulated

**IATA**

Not regulated

**Special Precautions for User**

No special precautions required

**SECTION 15. REGULATORY INFORMATION**

## 8-Chlorotheophylline

## International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
8-Chlorotheophylline	-	-	X	-	201-590-4	-	-	-	X	X	-	-

## National Regulations

## SECTION 16. OTHER INFORMATION

**Prepared By** Health, Safety and Environmental Department  
**Revision Date** 29-Apr-2024  
**Revision Summary** New emergency telephone response service provider.

## Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

**CAS** - Chemical Abstracts Service

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

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

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

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

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

## Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**SAFETY DATA SHEET****8-Chlorotheophylline**

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**Disclaimer**

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**End of Safety Data Sheet**