



## SAFETY DATA SHEET

### 8-Chlorotheophylline

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

#### SECTION 1: Identification of the substance/mixture and of the company/undertaking

##### 1.1. Product identifier

Product name	8-Chlorotheophylline
CAS number	85-18-7
EC number	201-590-4

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

Identified uses	For research purposes only.
Uses advised against	Not suitable for human consumption or veterinary purposes.

##### 1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
----------	---

##### 1.4. Emergency telephone number

+44 (0) 7769276927

#### SECTION 2: Hazards identification

##### 2.1. Classification of the substance or mixture

###### Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Acute Tox. 4 - H302
Environmental hazards	Not Classified

##### 2.2. Label elements

EC number	201-590-4
-----------	-----------

###### Hazard pictograms



Signal word	Warning
Hazard statements	H302 Harmful if swallowed.

## 8-Chlorotheophylline

<b>Precautionary statements</b>	P264 Wash contaminated skin thoroughly after handling.
	P270 Do not eat, drink or smoke when using this product.
	P301+P312 IF SWALLOWED: Call a POISON CENTRE/doctor if you feel unwell.
	P330 Rinse mouth.
	P501 Dispose of contents/ container in accordance with national regulations.

### 2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

<b>Product name</b>	8-Chlorotheophylline
<b>CAS number</b>	85-18-7
<b>EC number</b>	201-590-4
<b>Chemical formula</b>	C7H7ClN4O2

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

<b>General information</b>	If in doubt, get medical attention promptly. Show this Safety Data Sheet to the medical personnel.
<b>Inhalation</b>	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Loosen tight clothing such as collar, tie or belt. Get medical attention if symptoms are severe or persist.
<b>Ingestion</b>	Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on their side in the recovery position and ensure breathing can take place. Keep affected person under observation. Get medical attention if symptoms are severe or persist.
<b>Skin contact</b>	Rinse with water.
<b>Eye contact</b>	Remove any contact lenses and open eyelids wide apart. Rinse with water. Get medical attention if any discomfort continues.
<b>Protection of first aiders</b>	First aid personnel should wear appropriate protective equipment during any rescue.

### 4.2. Most important symptoms and effects, both acute and delayed

<b>General information</b>	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
<b>Inhalation</b>	A single exposure may cause the following adverse effects: Temporary irritation.
<b>Ingestion</b>	May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.
<b>Skin contact</b>	Prolonged contact may cause dryness of the skin.
<b>Eye contact</b>	May be slightly irritating to eyes.

### 4.3. Indication of any immediate medical attention and special treatment needed

<b>Notes for the doctor</b>	Treat symptomatically.
-----------------------------	------------------------

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

## 8-Chlorotheophylline

**Suitable extinguishing media** Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

**Unsuitable extinguishing media** Do not use water jet as an extinguisher, as this will spread the fire.

### 5.2. Special hazards arising from the substance or mixture

**Specific hazards** This product is toxic.

**Hazardous combustion products** Thermal decomposition or combustion products may include the following substances:  
Toxic gases or vapours.  
Carbon dioxide (CO<sub>2</sub>).  
Carbon monoxide (CO).  
Oxides of nitrogen.  
Hydrogen chloride (HCl).

### 5.3. Advice for firefighters

**Protective actions during firefighting** Avoid breathing fire gases or vapours. Evacuate area. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.

**Special protective equipment for firefighters** Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

## SECTION 6: Accidental release measures

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

**Personal precautions** Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material.

### 6.2. Environmental precautions

**Environmental precautions** Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.

### 6.3. Methods and material for containment and cleaning up

**Methods for cleaning up** Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Provide adequate ventilation. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

### 6.4. Reference to other sections

**Reference to other sections** For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

**Usage precautions** Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

## 8-Chlorotheophylline

### Advice on general occupational hygiene

Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

### 7.2. Conditions for safe storage, including any incompatibilities

#### Storage precautions

Store away from incompatible materials (see Section 10). Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

#### Storage class

Chemical storage.

### 7.3. Specific end use(s)

#### Specific end use(s)

The identified uses for this product are detailed in Section 1.2.

## SECTION 8: Exposure controls/Personal protection

### 8.1. Control parameters

#### Occupational exposure limits

STEL:

TWA:

### 8.2. Exposure controls

#### Protective equipment



#### Appropriate engineering controls

Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

#### Eye/face protection

Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses.

#### Hand protection

No specific hand protection recommended.

#### Other skin and body protection

Wear appropriate clothing to prevent repeated or prolonged skin contact.

#### Hygiene measures

Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.

#### Respiratory protection

Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.

#### Environmental exposure controls

Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

#### Appearance

Powder.

#### Colour

White/off-white.

## 8-Chlorotheophylline

Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	292°C/557.6°F
Initial boiling point and range	455°C/851°F
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	< 0.0000001 kPa @ 25°C/77°F
Vapour density	No information available.
Relative density	1.591 g/cm3
Solubility(ies)	Slightly soluble in water. Slightly soluble in the following materials: Chloroform. DMSO Methanol.
Partition coefficient	log Pow: -0.52
Auto-ignition temperature	No information available.
Decomposition Temperature	300°C/572°F

### 9.2. Other information

Molecular weight	214.61
------------------	--------

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Reactivity	See the other subsections of this section for further details.
------------	--

### 10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.
-----------	---

### 10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	No potentially hazardous reactions known.
------------------------------------	---

### 10.4. Conditions to avoid

Conditions to avoid	There are no known conditions that are likely to result in a hazardous situation.
---------------------	---

### 10.5. Incompatible materials

Materials to avoid	Strong oxidising agents.
--------------------	--------------------------

### 10.6. Hazardous decomposition products

## 8-Chlorotheophylline

<b>Hazardous decomposition products</b>	<p>Does not decompose when used and stored as recommended.</p> <p>Thermal decomposition or combustion products may include the following substances:</p> <p>Toxic gases or vapours.</p> <p>Carbon dioxide (CO<sub>2</sub>).</p> <p>Carbon monoxide (CO).</p> <p>Oxides of:</p> <p>Nitrogen.</p> <p>Hydrogen chloride (HCl).</p>
---	---

### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

##### Acute toxicity - oral

**Summary** Harmful if swallowed.

**Acute toxicity oral (LD<sub>50</sub> mg/kg)** 440.0

**Species** Rat

**ATE oral (mg/kg)** 440.0

##### Acute toxicity - dermal

**Summary** Based on available data the classification criteria are not met.

##### Acute toxicity - inhalation

**Summary** Based on available data the classification criteria are not met.

##### Skin corrosion/irritation

**Summary** Based on available data the classification criteria are not met.

##### Serious eye damage/irritation

**Summary** Based on available data the classification criteria are not met.

##### Respiratory sensitisation

**Summary** Based on available data the classification criteria are not met.

##### Skin sensitisation

**Summary** Based on available data the classification criteria are not met.

##### Germ cell mutagenicity

**Summary** Based on available data the classification criteria are not met.

##### Carcinogenicity

**Summary** Based on available data the classification criteria are not met.

**IARC carcinogenicity** None of the ingredients are listed or exempt.

##### Reproductive toxicity

**Summary** Based on available data the classification criteria are not met.

##### Specific target organ toxicity - single exposure

**Summary** Based on available data the classification criteria are not met.

##### Specific target organ toxicity - repeated exposure

**Summary** Based on available data the classification criteria are not met.

##### Aspiration hazard

**Summary** Not relevant. Solid.

## 8-Chlorotheophylline

<b>General information</b>	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
<b>Inhalation</b>	A single exposure may cause the following adverse effects: Temporary irritation.
<b>Ingestion</b>	May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.
<b>Skin contact</b>	Prolonged contact may cause dryness of the skin.
<b>Eye contact</b>	May be slightly irritating to eyes.
<b>Route of exposure</b>	Ingestion Inhalation Skin and/or eye contact
<b>Target organs</b>	No specific target organs known.

### SECTION 12: Ecological information

<b>Ecotoxicity</b>	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.
--------------------	---

#### 12.1. Toxicity

##### Acute aquatic toxicity

<b>Summary</b>	Based on available data the classification criteria are not met.
----------------	--

##### Chronic aquatic toxicity

<b>Summary</b>	Based on available data the classification criteria are not met.
----------------	--

#### 12.2. Persistence and degradability

<b>Persistence and degradability</b>	The degradability of the product is not known.
--------------------------------------	--

#### 12.3. Bioaccumulative potential

<b>Bioaccumulative potential</b>	No data available on bioaccumulation.
----------------------------------	---------------------------------------

<b>Partition coefficient</b>	log Pow: -0.52
------------------------------	----------------

#### 12.4. Mobility in soil

<b>Mobility</b>	No data available.
-----------------	--------------------

#### 12.5. Results of PBT and vPvB assessment

#### 12.6. Other adverse effects

<b>Other adverse effects</b>	None known.
------------------------------	-------------

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

<b>General information</b>	The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.
<b>Disposal methods</b>	Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

## 8-Chlorotheophylline

### SECTION 14: Transport information

**General** The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).

#### 14.1. UN number

Not applicable.

#### 14.2. UN proper shipping name

Not applicable.

#### 14.3. Transport hazard class(es)

No transport warning sign required.

#### 14.4. Packing group

Not applicable.

#### 14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

#### 14.6. Special precautions for user

Not applicable.

#### 14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Not applicable.

Annex II of MARPOL 73/78

and the IBC Code

### SECTION 15: Regulatory information

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

##### **National regulations**

Health and Safety at Work etc. Act 1974 (as amended).

The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment

Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].

EH40/2005 Workplace exposure limits.

#### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

#### Inventories

##### **EU - EINECS/ELINCS**

None of the ingredients are listed or exempt.

### SECTION 16: Other information



## 8-Chlorotheophylline

<b>Abbreviations and acronyms used in the safety data sheet</b>	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
	ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
	RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
	IATA: International Air Transport Association.
	ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.
	IMDG: International Maritime Dangerous Goods.
	CAS: Chemical Abstracts Service.
	ATE: Acute Toxicity Estimate.
	LC50: Lethal Concentration to 50 % of a test population.
	LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).
	EC <sub>50</sub> : 50% of maximal Effective Concentration.
	PBT: Persistent, Bioaccumulative and Toxic substance.
	vPvB: Very Persistent and Very Bioaccumulative.
<b>Classification abbreviations and acronyms</b>	Acute Tox. = Acute toxicity
<b>Classification procedures according to SI 2019 No. 720</b>	Acute Tox. 4 - H302: : Expert judgement.
<b>Training advice</b>	Only trained personnel should use this material.
<b>Revision date</b>	22/05/2023
<b>Revision</b>	1
<b>SDS number</b>	2291
<b>Hazard statements in full</b>	H302 Harmful if swallowed.

This 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. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.