

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

### 1.1. Product identifier

Product Description:	<b>1-n-Hexyltheobromine</b>
Cat No. :	<b>L13597</b>
CAS No	1028-33-7
Molecular Formula	C13 H20 N4 O2

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

Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

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

#### Company

Thermo Fisher (Kandel) GmbH  
Erlenbachweg 2, 76870 Kandel, Germany  
Tel: +49 (0) 721 84007 280  
Fax: +49 (0) 721 84007 300

**Swiss distributor - Fisher Scientific AG**  
Neuhofstrasse 11, CH 4153 Reinach  
Tel: +41 (0) 56 618 41 11  
<https://www.fishersci.ch/ch/en/customer-help-support/forms/email-us.html>

#### E-mail address

[begel.sdsdesk@thermofisher.com](mailto:begel.sdsdesk@thermofisher.com)

### 1.4. 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

customers in Switzerland:  
Tox Info Suisse Emergency Number: **145 (24hr)**  
Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)  
Chemtrec (24h) Toll-Free: 0800 564 402  
Chemtrec Local: +41-43 508 20 11 (Zurich)

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

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## Physical hazards

Based on available data, the classification criteria are not met

## Health hazards

Based on available data, the classification criteria are not met

## Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements

None required

## 2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - Regulation (EC) No 1272/2008
Pentifylline	1028-33-7	EEC No. 213-842-0	<=100	-

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
<b>Inhalation</b>	Remove to fresh air. Get medical attention immediately if symptoms occur.
<b>Self-Protection of the First Aider</b>	No special precautions required.

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

None reasonably foreseeable.

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

Notes to Physician

Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

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

No information available.

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

Thermal decomposition can lead to release of irritating gases and vapors.

#### **Hazardous Combustion Products**

None under normal use conditions.

### 5.3. Advice 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

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

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

### 6.2. Environmental precautions

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

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

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation. Avoid dust formation.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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

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

**Technical Rules for Hazardous Substances (TRGS) 510**  
**Storage Class (LGK) (Germany)**

Storage Class/LGK 11

**Switzerland - Storage of hazardous substances**

<https://www.kvu.ch/de/themen/stoffe-und-produkte>  
<https://www.kvu.ch/fr/themes/substances-et-produits>  
<https://www.kvu.ch/it/temi/sostanze-e-prodotti> Storage class - SC 11/13

## **7.3. Specific end use(s)**

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1. Control parameters**

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **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

#### **Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

No information available

#### **Predicted No Effect Concentration (PNEC)**

No information available.

### **8.2. Exposure controls**

#### **Engineering Measures**

None under normal use conditions.

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## Personal protective equipment

### Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

### Hand Protection

Protective gloves

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

### Skin and body protection

Long sleeved clothing.

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

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

**Recommended Filter type:** Particle filter

### Small scale/Laboratory use

Maintain adequate ventilation

### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

Physical State	Solid	
Appearance	White	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	80 - 81 °C / 176 - 177.8 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	No information available	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	Not applicable	Solid
Water Solubility	Insoluble in water	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

### 9.2. Other information

Molecular Formula	C13 H20 N4 O2
Molecular Weight	264.33

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Evaporation Rate Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

**10.1. Reactivity** None known, based on information available

**10.2. Chemical stability** Stable under normal conditions.

**10.3. Possibility of hazardous reactions**

**Hazardous Polymerization** No information available.  
**Hazardous Reactions** None under normal processing.

**10.4. Conditions to avoid** Incompatible products. Excess heat.

**10.5. Incompatible materials** None known.

**10.6. Hazardous decomposition products** None under normal use conditions.

## SECTION 11: TOXICOLOGICAL INFORMATION

**11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008**

**Product Information**

**(a) acute toxicity;**  
    **Oral** No data available  
    **Dermal** No data available  
    **Inhalation** No data available

**(b) skin corrosion/irritation;** No data available

**(c) serious eye damage/irritation;** No data available

**(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;** No data available

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(i) STOT-repeated exposure; No data available  
Target Organs No information available.

(j) aspiration hazard; Not applicable  
Solid

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

## 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

**Ecotoxicity effects** Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

### 12.2. Persistence and degradability

**Persistence** Insoluble in water.

**12.3. Bioaccumulative potential** May have some potential to bioaccumulate

### 12.4. Mobility in soil

Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility.

### 12.5. Results of PBT and vPvB assessment

No data available for assessment.

### 12.6. Endocrine disrupting properties

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

### 12.7. Other adverse effects

**Persistent Organic Pollutant** This product does not contain any known or suspected substance  
**Ozone Depletion Potential** This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

**Waste from Residues/Unused Products** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

**Contaminated Packaging** Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.

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<b>European Waste Catalogue (EWC)</b>	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used.
<b>Switzerland - Waste Ordinance</b>	Disposal should be in accordance with applicable regional, national and local laws and regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance, ADWO) SR 814.600 <a href="https://www.fedlex.admin.ch/eli/cc/2015/891/en">https://www.fedlex.admin.ch/eli/cc/2015/891/en</a>

## SECTION 14: TRANSPORT INFORMATION

**IMDG/IMO** Not regulated

14.1. UN number  
14.2. UN proper shipping name  
14.3. Transport hazard class(es)  
14.4. Packing group

**ADR** Not regulated

14.1. UN number  
14.2. UN proper shipping name  
14.3. Transport hazard class(es)  
14.4. Packing group

**IATA** Not regulated

14.1. UN number  
14.2. UN proper shipping name  
14.3. Transport hazard class(es)  
14.4. Packing group

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### **International Inventories**

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Pentifylline	1028-33-7	213-842-0	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Pentifylline	1028-33-7	-	-	-	-	-	-	-

**Legend:** X - Listed '-' - Not Listed

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

**Authorisation/Restrictions according to EU REACH**

Not applicable



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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)
Pentifylline	1028-33-7	-	-	-

## Seveso III Directive (2012/18/EC)

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
Pentifylline	1028-33-7	Not applicable	Not applicable

## Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

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

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** Water endangering class = 3 (self classification)

## Swiss Regulations

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

#### 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

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer  
Predicted No Effect Concentration (PNEC)

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**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code  
**OECD** - Organisation for Economic Co-operation and Development  
**BCF** - Bioconcentration factor

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

**Training Advice**

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

**Prepared By**

Health, Safety and Environmental Department

**Revision Date**

14-Feb-2024

**Revision Summary**

New emergency telephone response service provider.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No 1907/2006 .**

**For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2, Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and Preparations).**

**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 Safety Data Sheet**