

ALFAAL13597

## 1-n-Hexyltheobromine

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

<b>产品说明:</b> <b>Product Description:</b>	<b>1-正-己基可可碱</b> <b>1-n-Hexyltheobromine</b>
<b>Cat No. :</b>	<b>L13597</b>
<b>CAS No</b>	1028-33-7
<b>Molecular Formula</b>	C13 H20 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> Solid	<b>Appearance</b> White	<b>Odor</b> No information available
<b>Emergency Overview</b> The product contains no substances which at their given concentration are considered to be hazardous to health.		

#### Classification of the substance or mixture

Based on available data, the classification criteria are not met

#### Label Elements

None required

#### Physical and Chemical Hazards

None identified.

#### Health Hazards

The product contains no substances which at their given concentration are considered to be hazardous to health.

#### Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil.

This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
Pentifylline	1028-33-7	<=100

**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 plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.

**Inhalation**

Remove to fresh air. Get medical attention immediately if symptoms occur.

**Ingestion**

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

**Most important symptoms and effects**

None reasonably foreseeable.

**Self-Protection of the First Aider**

No special precautions required.

**Notes to Physician**

Treat symptomatically.

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

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

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

No information available.

**Specific Hazards Arising from the Chemical**

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

**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. 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. Avoid dust formation.

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7. HANDLING AND STORAGE

### Handling

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

### Storage

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

### 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

### Exposure Controls

### Engineering Measures

None under normal use conditions.

### 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				

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** Long sleeved clothing

**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

**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>	Solid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	80 - 81 °C / 176 - 177.8 °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
<b>Evaporation Rate</b>	Not applicable	Solid
<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	
<b>Bulk Density</b>	No data available	
<b>Water Solubility</b>	Insoluble in water	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid
<b>Explosive Properties</b>	No information available	
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C13 H20 N4 O2	
<b>Molecular Weight</b>	264.33	

## SECTION 10. STABILITY AND REACTIVITY

**Stability** Stable under normal conditions.

**Hazardous Reactions** None under normal processing.

**Hazardous Polymerization** No information available.

**Conditions to Avoid** None known.

**Materials to avoid** No information available.

**Hazardous Decomposition Products** None under normal use conditions.

## SECTION 11. TOXICOLOGICAL INFORMATION

### Product Information

(a) acute toxicity;

(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
(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

**SECTION 12. ECOLOGICAL INFORMATION**

Ecotoxicity effects	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
Persistence and Degradability	
Persistence	Insoluble in water.
Bioaccumulative Potential	May have some potential to bioaccumulate
Mobility in soil	Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility
Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
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**

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.
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<b>Contaminated Packaging</b>	Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used.

## 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

## 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
Pentifylline	-	-		-	213-842-0	-	-	-	-		-	-

## National Regulations

## SECTION 16. OTHER INFORMATION

**Prepared By** Health, Safety and Environmental Department  
**Revision Date** 01-May-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.

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

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**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

**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**