Chemical Safety Data Sheet MSDS / SDS

1-N-HEXYLTHEOBROMINE

Revision Date:2024-11-23 Revision Number:1

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

Product identifier

Product name	: 1-N-HEXYLTHEOBROMINE				
CBnumber	: CB3219560				
CAS	: 1028-33-7				
EINECS Number	: 213-842-0				
Synonyms	: Pentifylline,1-hexyl-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione				
Relevant identified uses of the substance or mixture and uses advised against					
Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.				
Uses advised against	: none				
Company Identification					
Company	: Chemicalbook				
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing				
Telephone	: 400-158-6606				

SECTION 2: Hazards identification

Classification of the substance or mixture Not classified. Label elements Pictogram(s) Signal word Warning Hazard statement(s) H302 Harmful if swallowed Precautionary statement(s) P264 Wash hands thoroughly after handling. P264 Wash skin thouroughly after handling. P270 Do not eat, drink or smoke when using this product. P330 Rinse mouth. Prevention

1

Response

none

Storage

none

Disposal

none

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1-N-HEXYLTHEOBROMINE
Synonyms	: Pentifylline,1-hexyl-3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione
CAS	: 1028-33-7
EC number	: 213-842-0
MF	: C13H20N4O2
MW	: 264.32

SECTION 4: First aid measures

Description of first aid measures

lf inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms and effects, both acute and delayed

no data available

Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

Extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

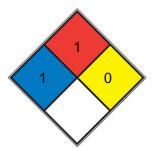
Specific Hazards Arising from the Chemical

no data available

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704



		1 Exposure would cause irritation with only minor residual injury (e.g. acetone, sodium bromate, potassium chloride)	
FIRE	1	Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. <u>mineral oil</u> , ammonia)	
REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)	
SPEC. HAZ.			

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use sparkproof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the riskelimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The

selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	no data available
Colour	no data available
Odour	no data available
Melting point/freezing point	80-81°C
Boiling point or initial boiling point and	452.5°C at 760mmHg
boiling range	
Flammability	no data available
Lower and upper explosion	no data available

limit/flammability limit

Flash point	227.5°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
рН	no data available
Kinematic viscosity	no data available
Solubility	no data available
Partition coefficient n-octanol/water	no data available
Vapour pressure	2.23E-08mmHg at 25°C
Density and/or relative density	1.23g/cm3
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available Toxicity to daphnia and other aquatic invertebrates: no data available Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: no data available IMDG: no data available IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available IMDG: no data available IATA: no data available

Transport hazard class(es)

ADR/RID: no data available IMDG: no data available IATA: no data available

Packing group, if applicable

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Environmental hazards

ADR/RID: No IMDG: No IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS) Listed. **EC Inventory** Listed. United States Toxic Substances Control Act (TSCA) Inventory Not Listed. China Catalog of Hazardous chemicals 2015 Not Listed. New Zealand Inventory of Chemicals (NZIoC) Not Listed. PICCS Not Listed. **Vietnam National Chemical Inventory** Not Listed. IECSC Not Listed. Korea Existing Chemicals List (KECL) Not Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road RID: Regulation concerning the International Carriage of Dangerous Goods by Rail IMDG: International Maritime Dangerous Goods IATA: International Air Transportation Association TWA: Time Weighted Average STEL: Short term exposure limit LC50: Lethal Concentration 50% LD50: Lethal Dose 50% EC50: Effective Concentration 50%

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?

pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.