

MATERIAL SAFETY DATA SHEET (MSDS)

1-N-Hexyltheobromine | Prepared in accordance with the Globally Harmonised System (GHS Rev. 9) and REACH Regulation (EC) No. 1907/2006 Annex II.

SECTION 1: IDENTIFICATION OF THE SUBSTANCE AND OF THE SUPPLIER

Product Name	1-N-Hexyltheobromine
C.A.S. Number	1028-33-7
Product Category	Fine & Research Chemicals
Product Group	Research Chemicals
Grade / Standard	98% min.
Identified Uses	Research, analysis and fine chemical synthesis. Industrial and professional use.
Uses Advised Against	Any application not described above without prior written confirmation from the supplier.
Supplier	Scapex Exports Pvt. Ltd., 830, 8th Floor, Sun Gravitas, Times of India Road, Shyamal, Ahmedabad – 380015, Gujarat, India
Telephone / E-mail	+91 9925522674 info@scapexexports.com
Emergency Telephone	+91 9925522674 (Mon–Sat, 09:30–18:30 IST)
MSDS Number	SCX/MSDS/5A5DF8

SECTION 2: HAZARDS IDENTIFICATION

GHS Classification	Not classified as dangerous for transport
Signal Word	WARNING
Pictograms	Exclamation mark

Hazard Statements

- H315 — Causes skin irritation.
- H319 — Causes serious eye irritation.

Precautionary Statements

- P101 If medical advice is needed, have product container or label at hand.
- P102 Keep out of reach of children.
- P262 Do not get in eyes, on skin, or on clothing.
- P264 Wash hands thoroughly after handling.
- P280 Wear protective gloves and eye protection.
- P302+P352 IF ON SKIN: Wash with plenty of water.
- P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes.
- P337+P313 If eye irritation persists: Get medical advice / attention.

SECTION 3: COMPOSITION / INFORMATION ON INGREDIENTS

Chemical Identity	1-N-Hexyltheobromine
C.A.S. Number	1028-33-7
Concentration / Grade	98% min.
Impurities	No impurities present at concentrations that alter the classification of the product.

SECTION 4: FIRST-AID MEASURES

Inhalation	Remove the casualty to fresh air and keep at rest in a position comfortable for breathing. If breathing is difficult, give oxygen. If breathing has stopped, give artificial respiration. Obtain medical attention.
Skin Contact	Remove contaminated clothing and shoes immediately. Wash the affected area with plenty of soap and water for at least 15 minutes. Obtain medical attention if irritation develops or persists.
Eye Contact	Rinse immediately with plenty of water for at least 15 minutes, holding the eyelids open. Remove contact lenses if present and easy to do. Obtain immediate medical attention.
Ingestion	Do NOT induce vomiting. Rinse the mouth with water. Never give anything by mouth to an unconscious person. Obtain immediate medical attention and show this Material Safety Data Sheet (MSDS).
Note to Physician	Treat symptomatically. No specific antidote is known.

SECTION 5: FIRE-FIGHTING MEASURES

Suitable Extinguishing Media	Water spray, dry chemical powder, carbon dioxide (CO ₂) or alcohol-resistant foam.
Unsuitable Extinguishing Media	High-pressure water jet.
Specific Hazards	Thermal decomposition may generate irritating and toxic gases. Containers may rupture when heated.
Advice for Fire-fighters	Wear self-contained breathing apparatus and full protective clothing. Prevent fire-fighting water entering drains or watercourses.

SECTION 6: ACCIDENTAL RELEASE MEASURES

Personal Precautions	Evacuate unnecessary personnel. Ensure adequate ventilation. Wear the personal protective equipment described in Section 8. Eliminate all ignition sources where the product is flammable.
Environmental Precautions	Prevent entry into drains, sewers, surface water and groundwater. Notify the relevant authorities if release to the environment occurs.
Containment & Cleaning	Contain the spill with an inert absorbent (dry sand, earth or vermiculite). Collect into a labelled, closed container for disposal. Do not use combustible absorbents such as sawdust where the product is an oxidiser. Ventilate the area and wash the spill site after material pick-up.

SECTION 7: HANDLING AND STORAGE

Precautions for Handling	Use only in well-ventilated areas. Avoid contact with skin, eyes and clothing. Avoid the formation and inhalation of dust, mist or vapour. Do not eat, drink or smoke in the work area. Wash thoroughly after handling.
Conditions for Storage	Store in the original, tightly closed container in a cool, dry, well-ventilated place away from direct sunlight and heat. Keep away from incompatible materials listed in Section 10. Store in a bonded area where liquids are held.
Packaging Materials	Use only the original packaging or an equivalent material approved for this product.

SECTION 8: EXPOSURE CONTROLS / PERSONAL PROTECTION

Occupational Exposure Limits	Refer to the national occupational exposure limits applicable in the country of use. Where no limit is established, maintain airborne concentrations as low as reasonably practicable.
Engineering Controls	Provide local exhaust ventilation at points of dust, mist or vapour generation. Provide eyewash stations and safety showers close to the work station.

Eye / Face Protection	Chemical safety goggles to EN 166 / IS 5983. A face shield is required where splashing is possible.
Skin Protection	Chemical-resistant gloves to EN 374 (nitrile or butyl rubber, thickness and breakthrough time selected for the task). Chemical-resistant apron, suit and boots as required by the task.
Respiratory Protection	Where ventilation is insufficient, use an approved respirator with a particulate filter (P2/P3) for dusts or an appropriate vapour cartridge for solvents.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice. Remove and wash contaminated clothing before re-use.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Appearance as per specification
Odour	Characteristic
Physical State	Solid
pH	See product specification
Melting / Freezing Point	See product specification
Boiling Point / Range	See product specification
Flash Point	Not applicable
Relative Density	See product specification
Solubility	See product specification
Vapour Pressure	See product specification
Purity / Assay	98% min.

SECTION 10: STABILITY AND REACTIVITY

Reactivity	Stable under the recommended handling and storage conditions.
Chemical Stability	Stable under normal ambient conditions.
Possibility of Hazardous Reactions	None known under recommended conditions of use.
Conditions to Avoid	Heat, direct sunlight, moisture, ignition sources and mechanical damage to packaging.
Incompatible Materials	Strong oxidising agents, strong acids and strong bases.
Hazardous Decomposition Products	Oxides of carbon and other toxic fumes on thermal decomposition.

SECTION 11: TOXICOLOGICAL INFORMATION

Likely Routes of Exposure	Inhalation, skin contact, eye contact and ingestion.
Acute Toxicity	Product-specific LD50/LC50 data are available from the manufacturer on request.
Symptoms and Effects	Causes skin irritation, Causes serious eye irritation.
Carcinogenicity	Not classified as carcinogenic.
Reproductive Toxicity	Not classified for reproductive toxicity.
Germ Cell Mutagenicity	Not classified.
STOT — Single / Repeated Exposure	Not classified.

SECTION 12: ECOLOGICAL INFORMATION

Aquatic Toxicity	No significant ecotoxicity expected at normal use concentrations.
Persistence and Degradability	Data not available for this product. Assess against local discharge consent limits before release.
Bioaccumulative Potential	Data not available.
Mobility in Soil	Data not available.
Other Adverse Effects	Do not allow the product to enter drains, sewers or watercourses.

SECTION 13: DISPOSAL CONSIDERATIONS

Waste Treatment	Dispose of the product and its container through an authorised waste treatment or disposal facility, in accordance with local, state and national regulations. Do not discharge to drains or the environment.
Contaminated Packaging	Empty containers retain product residue. Triple-rinse where appropriate and offer for approved reconditioning or disposal. Do not re-use containers for other purposes.

SECTION 14: TRANSPORT INFORMATION

UN Number	Not regulated
UN Proper Shipping Name	Not applicable
Transport Hazard Class	Not applicable
Packing Group	Not applicable
Marine Pollutant	No
IMDG / IATA / ADR	Not classified as dangerous goods for transport by sea, air or road.

SECTION 15: REGULATORY INFORMATION

Classification System	Globally Harmonised System (GHS Rev. 9); CLP Regulation (EC) No. 1272/2008.
EU REACH	Registration status is held by the manufacturer. A REACH statement is available from Scapex Exports on request.
India	Manufacture, Storage and Import of Hazardous Chemicals Rules; Chemical Accidents (Emergency Planning, Preparedness and Response) Rules, as applicable.
Chemical Safety Assessment	A chemical safety assessment has not been carried out by Scapex Exports for this product.

SECTION 16: OTHER INFORMATION

Basis of Classification	Classification in Section 2 has been assigned on the basis of the chemical class of the product and the standard commercial grade supplied. Where the manufacturer of a particular batch publishes a different classification, the manufacturer's classification governs.
Full Text of H-statements	H315: Causes skin irritation.; H319: Causes serious eye irritation.
Revision	Revision 1 — first issue
Prepared by	Quality Assurance, Scapex Exports Pvt. Ltd.

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