Pfaltz & Bauer
RARE AND FINE CHEMICALS
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SAFETY DATA SHEET

SECTION 1: CHEMICAL PRODUCT and COMPANY IDENTIFICATION

Product Name:	Theobromine 99%
Product Code:	T09510
Supplier:	Pfaltz & Bauer, Inc. 172 E. Aurora Street Waterbury, CT 06708 USA
Phone:	203-574-0075
FAX:	203-574-3181
Emergency Phone:	INFOTRAC, US: 1-800-535-5053 INFOTRAC, INTERNATIONAL: +1-352-323-3500

SECTION 2: HAZARDS IDENTIFICATION

Statement of Hazard:	Irritant, Respiratory irritant
Acute Health Hazard:	Irritant to eyes, skin, mucous membranes and respiratory system. May be harmful by ingestion, skin absorption and inhalation.
Chronic Health Hazard:	Not Available
HMIS Rating:	H: 1 F: 0 P: 0
NFPA Rating:	H: 1 F: 0 R: 0

To the best of our knowledge, the toxicological properties of this chemical have not been thoroughly investigated. Use appropriate procedures and precautions to prevent or minimize exposure.

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS):

Acute toxicity, dermal (Category 4), H312
Acute toxicity, inhalation (Category 4), H332
Acute toxicity, oral (Category 4), H302
Serious eye damage/eye irritation (Category 2B), H320
Skin corrosion/irritation (Category 2), H315
Specific target organ toxicity, single exposure; Respiratory tract irritation (Category 3), H335

Pictogram:

Signal Word:	Warning
Hazard Statement(s):	H302 Harmful if swallowed. H312 Harmful in contact with skin. H315 Causes skin irritation. H320 Causes eye irritation. H332 Harmful if inhaled. H335 May cause respiratory irritation.
Precautionary Statement(s):	P261 Avoid breathing dust/fume/gas/mist/vapors/spray. P280 Wear protective gloves/protective clothing/eye protection/face protection. P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell. P302+P352 IF ON SKIN: wash with plenty of soap and water. P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing. P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P332+P313 IF SKIN irritation occurs: Get medical advice/attention.

SECTION 3: COMPOSITION/INFORMATION on INGREDIENTS

Chemical Name:	Theobromine 99%
Synonyms:	2,6-Dihydroxy-3,7-dimethylpurine; 3,7-Dimethylxanthine
CAS Number:	83-67-0
MDL Number:	MFCD00022830
EINECS Number:	201-494-2
Beilstein Registry Number:	16464
Molecular Formula:	$C_7H_8N_4O_2$
Molecular Weight:	180.17
Content:	As specified in product name.

SECTION 4: FIRST AID MEASURES

Eye Contact:	Flush eyes with large amounts of water for fifteen minutes. Separate eyelids with fingers. If irritation persists, seek medical attention.
Skin Contact:	Wash skin with soap and water. If irritation persists, seek medical attention.
Ingestion:	Do not induce vomiting. Seek medical attention.
Inhalation:	Move to a fresh air environment. Contact a physician if breathing becomes difficult.

SECTION 5: FIRE FIGHTING MEASURES

Flash Point (ºC):	Not Available
Explosion Limits:	Not Available
Auto Ignition Temperature (ºC):	Not Available
Extinguishing Media:	Carbon dioxide, dry chemical powder, alcohol-resistant foam, or water spray
Protective Equipment:	Wear self-contained respirator and fully protective impervious suit.
Specific Hazards:	May emit hazardous fumes under fire conditions.

SECTION 6: ACCIDENTAL RELEASE MEASURES

Personal Protection:	Wear a self-contained breathing apparatus, rubber boots and gloves, and disposable coveralls. Dispose of coveralls after use. Remove from ignition sources if safe to do so. Follow emergency response plan and contact proper authorities if needed. Keep unprotected persons away.
Environmental Protection:	Keep spills out of sewers and bodies of water. Dike and contain the spill with inert material. Absorb on sand, vermiculite or diatomite. Transfer material to a container for disposal or recovery. Ventilate area and wash spill site after material pickup is complete.

SECTION 7: HANDLING and STORAGE

Handling and Storage:	Avoid breathing dust, vapor, mist or gas. Avoid contact with skin and eyes. Avoid prolonged or repeated exposure. Use only in a chemical fume hood. Open and handle container with care. Keep ignition sources away. Store in a tightly closed container in a dry, well-ventilated place. Store under inert gas. Store under nitrogen.
Sensitivities:	Air

Storage Temperature (ºC): 15 to 30

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

Engineering Controls: Use product in a well ventilated area or under a fume hood. Use proper lab equipment while handling this product. Keep away from incompatible materials for possible risk of hazardous reaction.

Eye Protection: Wear appropriate protective eyeglass or chemical safety goggles. Make sure that there is an eyewash station in your vicinity.

Skin Protection: Wear impervious gloves and protective clothing.

Respiratory Protection: Use a NIOSH approved respirator when exposure limits are exceeded or if irritation or other symptoms are experienced.

Exposure Limits:

Country	Source	Type	Value
USA	ACGIH	TWA	Not Available
USA	OSHA	STEL	Not Available
USA	OSHA	PEL	Not Available

SECTION 9: PHYSICAL and CHEMICAL PROPERTIES

Appearance: White solid

Odor: Not Available

Odor Threshold: Not Available

Flash Point (ºC): Not Available

Auto Ignition Temperature (ºC): Not Available

UEL % by Volume: Not Available

LEL % by Volume: Not Available

Melting Point (ºC): 345-350

Boiling Point (ºC): Not Available

Evaporation Rate: Not Available

pH Value: Not Available

Density (g/cm³):	1.50
Refractive Index (n^{20}_D):	Not Available
Viscosity:	Not Available
Solubility in Water:	Slightly soluble
Solubility in Other:	Slightly soluble in Ethanol
Vapor Pressure (mmHg):	Not Available
Vapor Density (Air=1):	Not Available

SECTION 10: STABILITY and REACTIVITY

Stability:	Stable under normal temperatures and pressures.
Incompatibility:	Not Available
Reactivity:	Product may react with incompatible materials to release other hazardous substances.
Conditions to Avoid:	Heat, flame, sparks, other ignition sources.
Hazardous Decomposition Products:	Carbon oxides, Nitrogen oxides

SECTION 11: TOXICOLOGICAL INFORMATION

RTECS Reference:	XH2275000
Target Organs:	Not Available
Toxicity Data:	Oral Rat LD_{50} mg/kg: 1265.00 Oral Mouse LD_{50} mg/kg: 837.00
Carcinogenicity:	National Toxicology Program (NTP) listed: Not Available International Agency for Research on Cancer (IARC) listed: Not Available
Potential Symptoms:	Not Available

SECTION 12: ECOLOGICAL INFORMATION

Toxicity: Not Available

SECTION 13: DISPOSAL CONSIDERATIONS

Contact a licensed professional waste disposal service. Dispose in a manner consistent with federal, state and local environmental regulations.

SECTION 14: TRANSPORT INFORMATION

DOT Shipping Name: Not D.O.T.-Regulated

IMDG Shipping Name: Not Regulated

Marine Pollutant: No

IATA Shipping Name: Not Regulated

SECTION 15: REGULATORY INFORMATION

United States

Toxic Substance Control Act (TSCA) listed: Yes

Superfund Amendments and Reauthorization Act (SARA 302) listed: No

Superfund Amendments and Reauthorization Act (SARA 311/312) listed: No

Superfund Amendments and Reauthorization Act (SARA 313) listed: No

European Union

European Inventory of Existing Chemical Substances (EINECS): 201-494-2

Canada

Canadian Domestic Substances List (DSL) listed: No

Canadian Non-Domestic Substances List (NDSL) listed: Yes

SECTION 16: OTHER INFORMATION

Date Prepared: 10/1/2018

The information above is presented in good faith. It is believed to be accurate and represents the best information currently available to us. However, we make no warranty with respect to such information and we assume no liability resulting from its use. The user should consider this information as a supplement to other information that may be available and make independent judgement to ensure proper use to protect the health and safety of employees and the environment. Pfaltz and Bauer shall not be held liable for any damage resulting from handling or from contact with the above product.