

Material Safety Data Sheet

Theobromine, 99%

ACC# 97168

Section 1 - Chemical Product and Company Identification

MSDS Name: Theobromine, 99%

Catalog Numbers: AC258821000, AC258822500

Synonyms: 3,7-Dimethylxanthine; 2,6-Dihydroxy-3,7-dimethylpurine; 3,7-Dihydro-3,7-dimethyl-1H-purine-2,6-dione. Theobromine is an alkaloid produced by plants of the genus Theobroma. Theobromine, the predominant methylxanthine in cocoa and chocolate, has been used as a bronchodilator.

Company Identification:

Acros Organics N.V.
One Reagent Lane
Fair Lawn, NJ 07410

For information in North America, call: 800-ACROS-01

For emergencies in the US, call CHEMTREC: 800-424-9300

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
83-67-0	Theobromine	99	201-494-2

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: white powder.

Caution! May cause eye, skin, and respiratory tract irritation. May be harmful if swallowed.

Target Organs: Cardiovascular system.

Potential Health Effects

Eye: May cause eye irritation.

Skin: May cause skin irritation. The toxicological properties of this material have not been fully investigated.

Ingestion: May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May be harmful if swallowed. Theobromine is the principle alkaloid in cocoa with activity similar to that of caffeine. It produces weak CNS stimulation, but is a more potent diuretic, cardiac stimulant, and coronary dilator than caffeine.

Inhalation: May cause respiratory tract irritation. May cause irritation of the mucous membranes.

Chronic: No information found.

Section 4 - First Aid Measures

Eyes: Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid immediately.

Skin: Get medical aid. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes.

Ingestion: Never give anything by mouth to an unconscious person. Get medical aid immediately. Do NOT induce vomiting. If conscious and alert, rinse mouth and drink 2-4 cupfuls of milk or water.

Inhalation: Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.

Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion.

Extinguishing Media: Use extinguishing media most appropriate for the surrounding fire.

Flash Point: Not applicable.

Autoignition Temperature: Not applicable.

Explosion Limits, Lower: Not available.

Upper: Not available.

NFPA Rating: (estimated) Health: 1; Flammability: 1; Instability: 0

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.

Spills/Leaks: Sweep up, then place into a suitable container for disposal. Provide ventilation.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Use with adequate ventilation. Minimize dust generation and accumulation. Avoid contact with eyes, skin, and clothing. Avoid breathing dust.

Storage: Keep container closed when not in use. Store in a cool, dry area away from incompatible substances.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use adequate ventilation to keep airborne concentrations low.

Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
Theobromine	none listed	none listed	none listed

OSHA Vacated PELs: Theobromine: No OSHA Vacated PELs are listed for this chemical.

Personal Protective Equipment

Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin: Wear appropriate protective gloves to prevent skin exposure.

Clothing: Wear appropriate protective clothing to minimize contact with skin.

Respirators: A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use.

Section 9 - Physical and Chemical Properties

Physical State: Powder

Appearance: white

Odor: None reported.

pH: Not available.

Vapor Pressure: Not available.

Vapor Density: Not available.

Evaporation Rate: Not available.

Viscosity: Not available.

Boiling Point: Not available.

Freezing/Melting Point: 375 deg C (sublimes 290-29)

Decomposition Temperature: Not available.

Solubility: slightly soluble

Specific Gravity/Density: Not available.

Molecular Formula: C₇H₈N₄O₂

Molecular Weight: 180.17

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.

Conditions to Avoid: Dust generation.

Incompatibilities with Other Materials: Strong oxidizing agents.

Hazardous Decomposition Products: Nitrogen oxides, carbon monoxide, carbon dioxide.

Hazardous Polymerization: Will not occur.

Section 11 - Toxicological Information

RTECS#:

CAS# 83-67-0: XH2275000

LD50/LC50:

CAS# 83-67-0:

Oral, mouse: LD50 = 837 mg/kg;

Oral, rat: LD50 = 1265 mg/kg;

Carcinogenicity:

CAS# 83-67-0: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information found

Teratogenicity: Teratogenic effects have occurred in experimental animals.

Reproductive Effects: Oral, rat: TDLo = 7500 mg/kg (male, 49 days pre-mating--reproductive system effects).

Mutagenicity: Mutagenic effects have occurred in experimental animals. Mutagenic effects have occurred in humans.

Neurotoxicity: No information found

Other Studies:

Section 12 - Ecological Information

No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

RCRA P-Series: None listed.

RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	Not regulated as a hazardous material	No information available.
Hazard Class:		
UN Number:		
Packing Group:		

Section 15 - Regulatory Information

US FEDERAL

TSCA

CAS# 83-67-0 is listed on the TSCA inventory.

Health & Safety Reporting List

None of the chemicals are on the Health & Safety Reporting List.

Chemical Test Rules

None of the chemicals in this product are under a Chemical Test Rule.

Section 12b

None of the chemicals are listed under TSCA Section 12b.

TSCA Significant New Use Rule

None of the chemicals in this material have a SNUR under TSCA.

CERCLA Hazardous Substances and corresponding RQs

None of the chemicals in this material have an RQ.

SARA Section 302 Extremely Hazardous Substances

None of the chemicals in this product have a TPQ.

SARA Codes

CAS # 83-67-0: delayed.

Section 313

No chemicals are reportable under Section 313.

Clean Air Act:

This material does not contain any hazardous air pollutants.

This material does not contain any Class 1 Ozone depleters.

This material does not contain any Class 2 Ozone depleters.

Clean Water Act:

None of the chemicals in this product are listed as Hazardous Substances under the CWA.

None of the chemicals in this product are listed as Priority Pollutants under the CWA.

None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:

None of the chemicals in this product are considered highly hazardous by OSHA.

STATE

CAS# 83-67-0 is not present on state lists from CA, PA, MN, MA, FL, or NJ.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

XN

Risk Phrases:

R 22 Harmful if swallowed.

Safety Phrases:

S 22 Do not breathe dust.

S 24/25 Avoid contact with skin and eyes.

WGK (Water Danger/Protection)

CAS# 83-67-0: 1

Canada - DSL/NDSL

CAS# 83-67-0 is listed on Canada's DSL List.

Canada - WHMIS

This product has a WHMIS classification of D2A.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

Section 16 - Additional Information

MSDS Creation Date: 7/12/1999

Revision #5 Date: 10/24/2005

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall Fisher be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if Fisher has been advised of the possibility of such damages.