

Theobromine

sc-203296

Material Safety Data Sheet



The Power to Question

Hazard Alert Code
Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

Theobromine

STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA



SUPPLIER

Santa Cruz Biotechnology, Inc.
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EMERGENCY

ChemWatch

Within the US & Canada: 877-715-9305

Outside the US & Canada: +800 2436 2255

(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS

C7-H8-N4-O2, "3, 7-dihydro-3, 7-dimethyl-1H-purine-2, 6-dione", "1H-purine, 2, 6-dione, 3, 7-dihydro-3, 7-dimethyl-", "theophylline isomer", "3, 7-dimethylxanthine", "xanthine, 3, 7-dimethyl", xantheose, Diurobromine, Santheose, "SC 15090", Teobromin, Theosalvose, Theostene, Thesal, Thesodate

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	2		
Body Contact:	0		Min/Nil=0 Low=1
Reactivity:	1		Moderate=2 High=3
Chronic:	2		Extreme=4

CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

Harmful if swallowed.

Possible risk of harm to the unborn child.

Possible risk of irreversible effects.

Limited evidence of a carcinogenic effect*.

* (limited evidence).

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ Accidental ingestion of the material may be harmful; animal experiments indicate that ingestion of less than 150 gram may be fatal or may produce serious damage to the health of the individual.

■ Ingestion of small amounts (100-300 mg) theobromine is not harmful and helps relieve mental fatigue, drowsiness and general inertia. Large doses (above 1 gram) may cause palpitation, excitement, insomnia, dizziness, headache and vomiting.

■ Xanthine derivatives may produce nausea, vomiting, anorexia, stomach pain, vomiting of blood and diarrhoea.

Protein in the urine, increased amounts of urine output, and increased excretion of renal tubular cells and red blood cells may also occur.

EYE

■ Although the material is not thought to be an irritant (as classified by EC Directives), direct contact with the eye may cause transient discomfort characterised by tearing or conjunctival redness (as with windburn).

Slight abrasive damage may also result.

SKIN

■ Skin contact is not thought to produce harmful health effects (as classified under EC Directives using animal models).

Systemic harm, however, has been identified following exposure of animals by at least one other route and the material may still produce health damage following entry through wounds, lesions or abrasions.

■ Open cuts, abraded or irritated skin should not be exposed to this material.

■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.

Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

■ The material is not thought to produce either adverse health effects or irritation of the respiratory tract following inhalation (as classified by EC Directives using animal models).

Nevertheless, adverse systemic effects have been produced following exposure of animals by at least one other route and good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.

■ Inhalation of theobromine may cause nose and throat irritation, coughing and chest discomfort.

The material may act as a stimulant on excessive inhalation.

■ Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.

If prior damage to the circulatory or nervous systems has occurred or if kidney damage has been sustained, proper screenings should be conducted on individuals who may be exposed to further risk if handling and use of the material result in excessive exposures.

CHRONIC HEALTH EFFECTS

■ There has been some concern that this material can cause cancer or mutations but there is not enough data to make an assessment.

■ Strong evidence exists that this substance may cause irreversible mutations (though not lethal) even following a single exposure.

Based on experience with animal studies, exposure to the material may result in toxic effects to the development of the foetus, at levels which do not cause significant toxic effects to the mother.

Laboratory (in vitro) and animal studies show, exposure to the material may result in a possible risk of irreversible effects, with the possibility of producing mutation.

Excessive consumption of beverages containing theobromine may cause headaches, irritability and symptoms of anxiety neurosis.

Concerns with excessive exposure to theobromine include possible reproductive effects to foetal craniofacial area, musculoskeletal system, possible bladder cancer (2 separate epidemiological studies), myocardial infarction and, to lesser degrees, constipation, palpitations, shortness of breath and depressed mental state.

Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung. Prime symptom is breathlessness; lung shadows show on X-ray.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
theobromine	83-67-0	>99

Section 4 - FIRST AID MEASURES

SWALLOWED

- IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY.
- For advice, contact a Poisons Information Centre or a doctor.
- Urgent hospital treatment is likely to be needed.
- In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition.

EYE

If this product comes in contact with the eyes:

- Wash out immediately with fresh running water.
- Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.
- Seek medical attention without delay; if pain persists or recurs seek medical attention.
- Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.

SKIN

If skin or hair contact occurs:

- Flush skin and hair with running water (and soap if available).
- Seek medical attention in event of irritation.

INHALED

- If fumes, aerosols or combustion products are inhaled remove from contaminated area.
- Other measures are usually unnecessary.

NOTES TO PHYSICIAN

- for poisons (where specific treatment regime is absent):

BASIC TREATMENT

- Establish a patent airway with suction where necessary.
- Watch for signs of respiratory insufficiency and assist ventilation as necessary.
- Administer oxygen by non-rebreather mask at 10 to 15 L/min.
- Monitor and treat, where necessary, for pulmonary oedema .

Treat symptomatically.

If ingested within 4 hours in amounts over 15 mg/kg, removal from the stomach by Ipecac syrup or gastric lavage is recommended.

Activated charcoal is probably useful within the first 4 hours.

Magnesium sulfate cathartic may be useful.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Not applicable.
Upper Explosive Limit (%):	Not available.
Specific Gravity (water=1):	Not available
Lower Explosive Limit (%):	Not available.

EXTINGUISHING MEDIA

- Foam.
- Dry chemical powder.
- BCF (where regulations permit).
- Carbon dioxide.

FIRE FIGHTING

- Alert Fire Brigade and tell them location and nature of hazard.
- Wear breathing apparatus plus protective gloves.
- Prevent, by any means available, spillage from entering drains or water courses.
- Use water delivered as a fine spray to control fire and cool adjacent area.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- Combustible solid which burns but propagates flame with difficulty; it is estimated that most organic dusts are combustible (circa

70%) - according to the circumstances under which the combustion process occurs, such materials may cause fires and / or dust explosions.

- Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust (420 micron or less) may burn rapidly and fiercely if ignited - particles exceeding this limit will generally not form flammable dust clouds.; once initiated, however, larger particles up to 1400 microns diameter will contribute to the propagation of an explosion.
- In the same way as gases and vapours, dusts in the form of a cloud are only ignitable over a range of concentrations; in principle, the concepts of lower explosive limit (LEL) and upper explosive limit (UEL).are applicable to dust clouds but only the LEL is of practical use; - this is because of the inherent difficulty of achieving homogeneous dust clouds at high temperatures (for dusts the LEL is often called the "Minimum Explosible Concentration", MEC)
- A dust explosion may release of large quantities of gaseous products; this in turn creates a subsequent pressure rise of explosive force capable of damaging plant and buildings and injuring people.

Combustion products include: carbon monoxide (CO), carbon dioxide (CO₂), nitrogen oxides (NO_x), other pyrolysis products typical of burning organic material.

May emit poisonous fumes.

FIRE INCOMPATIBILITY

- Avoid contamination with oxidising agents i.e. nitrates, oxidising acids, chlorine bleaches, pool chlorine etc. as ignition may result

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.
- Avoid contact with skin and eyes.
- Control personal contact by using protective equipment.

MAJOR SPILLS

Moderate hazard.

- CAUTION: Advise personnel in area.
- Alert Emergency Services and tell them location and nature of hazard.
- Control personal contact by wearing protective clothing.
- Prevent, by any means available, spillage from entering drains or water courses.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.

Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source.

- Do NOT cut, drill, grind or weld such containers.
- In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorisation or permit.

RECOMMENDED STORAGE METHODS

- Polyethylene or polypropylene container.
- Check all containers are clearly labelled and free from leaks.

STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

- theobromine: CAS:83-67-0

PERSONAL PROTECTION



RESPIRATOR

- Particulate. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

EYE

- Safety glasses with side shields
- Chemical goggles.
- Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lens or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience. Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59], [AS/NZS 1336 or national equivalent]

HANDS/FEET

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include:

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and
- dexterity

Experience indicates that the following polymers are suitable as glove materials for protection against undissolved, dry solids, where abrasive particles are not present.

- polychloroprene
- nitrile rubber
- butyl rubber
- fluorocautchouc

OTHER

- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.

ENGINEERING CONTROLS

■ Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.

The basic types of engineering controls are:

Process controls which involve changing the way a job activity or process is done to reduce the risk.

Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Solid.

Does not mix with water.

State	Divided solid	Molecular Weight	180.2
Melting Range (°F)	675(subl 290)	Viscosity	Not Applicable
Boiling Range (°F)	Not applicable	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	Not Available	pH (1% solution)	Not available
Decomposition Temp (°F)	Not available.	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available.	Vapour Pressure (mmHG)	Not applicable.
Upper Explosive Limit (%)	Not available.	Specific Gravity (water=1)	Not available

Lower Explosive Limit (%)	Not available.	Relative Vapour Density (air=1)	Not applicable.
Volatile Component (%vol)	Not applicable	Evaporation Rate	Not applicable

APPEARANCE

Odorless microcrystalline powder with bitter taste; does not mix well with water (1 gm in 2000 ml cold water). Freely soluble in dilute mineral acids and aqueous solutions of alkali hydroxides. Isomeric with theophylline.

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerisation will not occur.

STORAGE INCOMPATIBILITY

- Avoid strong acids, bases.
- Avoid reaction with oxidising agents

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

theobromine

TOXICITY AND IRRITATION

■ While theobromine and caffeine are similar in that they are related alkaloids, theobromine is weaker in both its inhibition of cyclic nucleotide phosphodiesterases and its antagonism of adenosine receptors. Therefore, theobromine has a lesser impact on the human central nervous system than caffeine.

The substance is classified by IARC as Group 3:

NOT classifiable as to its carcinogenicity to humans.

Evidence of carcinogenicity may be inadequate or limited in animal testing.

CARCINOGEN

Theobromine	International Agency for Research on Cancer (IARC) - Agents Reviewed by the IARC Monographs	Group 3
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Section 12 - ECOLOGICAL INFORMATION

No data

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
theobromine	HIGH	No Data Available	LOW	HIGH

Section 13 - DISPOSAL CONSIDERATIONS

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

- Containers may still present a chemical hazard/ danger when empty.
- Return to supplier for reuse/ recycling if possible.

Otherwise:

- If container can not be cleaned sufficiently well to ensure that residuals do not remain or if the container cannot be used to store the same product, then puncture containers, to prevent re-use, and bury at an authorised landfill.
- Where possible retain label warnings and MSDS and observe all notices pertaining to the product.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse

- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate. In most instances the supplier of the material should be consulted.

- DO NOT allow wash water from cleaning or process equipment to enter drains.
- It may be necessary to collect all wash water for treatment before disposal.
- In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first.
- Where in doubt contact the responsible authority.
- Recycle wherever possible.
- Consult manufacturer for recycling options or consult local or regional waste management authority for disposal if no suitable treatment or disposal facility can be identified.
- Dispose of by: burial in a land-fill specifically licenced to accept chemical and / or pharmaceutical wastes or Incineration in a licenced apparatus (after admixture with suitable combustible material)
- Decontaminate empty containers. Observe all label safeguards until containers are cleaned and destroyed.

Section 14 - TRANSPORTATION INFORMATION

NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: DOT, IATA, IMDG

Section 15 - REGULATORY INFORMATION



theobromine (CAS: 83-67-0) is found on the following regulatory lists;

"Canada - Alberta Ambient Air Quality Guidelines", "Canada - Alberta Ambient Air Quality Objectives", "Canada - British Columbia Occupational Exposure Limits", "Canada - Ontario Occupational Exposure Limits", "Canada - Quebec Permissible Exposure Values for Airborne Contaminants (English)", "Canada Domestic Substances List (DSL)", "Canada National Pollutant Release Inventory (NPRI)", "Canada Non-Domestic Substances List (NDSL)", "Canada Substances in Products Regulated Under the Food and Drugs Act (F&DA) That Were In Commerce between January 1, 1987 and September 13, 2001 (English)", "International Agency for Research on Cancer (IARC) - Agents Reviewed by the IARC Monographs", "OECD List of High Production Volume (HPV) Chemicals", "US - California Permissible Exposure Limits for Chemical Contaminants", "US - Michigan Exposure Limits for Air Contaminants", "US - Oregon Permissible Exposure Limits (Z-1)", "US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants", "US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants", "US Clean Air Act (CAA) National Ambient Air Quality Standards (NAAQS)", "US FDA Everything Added to Food in the United States (EAFUS)", "US Toxic Substances Control Act (TSCA) - Chemical Substance Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

- Limited evidence of a carcinogenic effect*.

* (limited evidence).

Denmark Advisory list for selfclassification of dangerous substances

Substance	CAS	Suggested codes
theobromine	83- 67- 0	Mut3; R68 Xn; R22

- Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

A list of reference resources used to assist the committee may be found at:

www.chemwatch.net/references.

- The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings.

- For detailed advice on Personal Protective Equipment, refer to the following U.S. Regulations and Standards:

OSHA Standards - 29 CFR:

1910.132 - Personal Protective Equipment - General requirements

1910.133 - Eye and face protection

1910.134 - Respiratory Protection

1910.136 - Occupational foot protection
1910.138 - Hand Protection
Eye and face protection - ANSI Z87.1
Foot protection - ANSI Z41
Respirators must be NIOSH approved.

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