



TCI AMERICA

SAFETY DATA SHEET

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Revision number: 3
Revision date: 05/17/2016

1. IDENTIFICATION

Product name: 1-(3-Chloropropyl)theobromine
Product code: C1103

Product use: For laboratory research purposes.
Restrictions on use: Not for drug or household use.

Company:
TCI America
9211 N. Harborage Street
Portland, OR 97203 U.S.A.
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Emergency telephone number:
Chemical Emergencies:
TCI America (8:00am - 5:00pm) PST
+1-503-286-7624
Transportation Emergencies:
Chemtrec 24-Hour
+1-800-424-9300 (U.S.A.)
+1-703-527-3887 (International)
Responsible department:
TCI America
Environmental Health Safety and Security
+1- 503-286-7624

2. HAZARD(S) IDENTIFICATION

OSHA Haz Com: CFR 1910.1200: Acute Toxicity - Oral [Category 4]

Signal word: Warning!

Hazard Statement(s): Harmful if swallowed

Pictogram(s) or Symbol(s):



Precautionary Statement(s):

[Prevention]
[Response]
[Storage]
[Disposal]

Do not eat, drink or smoke when using this product. Wash hands and face thoroughly after handling.
If swallowed: Immediately call a poison center or doctor. Rinse mouth.
None
Dispose of contents and container in accordance with US EPA guidelines for the classification and determination of hazardous waste listed in 40 CFR 261.3. (See Section 13)

3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance/Mixture: Substance
Components: 1-(3-Chloropropyl)theobromine
Percent: >97.0%(HPLC)(T)
CAS Number: 74409-52-2
Molecular Weight: 256.69
Chemical Formula: $C_{10}H_{13}ClN_4O_2$
Synonyms: 1-(3-Chloropropyl)-3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione , 1-(3-Chloropropyl)-3,7-dimethylxanthine

4. FIRST-AID MEASURES

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Inhalation:	Call a poison center or doctor if you feel unwell. Move victim to fresh air. Give artificial respiration if victim is not breathing. Administer oxygen if breathing is difficult. Keep victim warm and quiet. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
Skin contact:	Call a poison center or doctor if you feel unwell. Remove and isolate contaminated clothing and shoes. In case of contact with substance, immediately flush skin with running water for at least 20 minutes. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
Eye contact:	If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper eyelids. If eye irritation persists get medical advice/attention. Move victim to fresh air. Check for and remove any contact lenses. Keep victim warm and quiet. Treat symptomatically and supportively. Effects of exposure to substance may be delayed. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
Ingestion:	Harmful if swallowed. If swallowed, seek medical advice immediately and show the container or label. Do not use mouth-to-mouth method if victim ingested the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Loosen tight clothing such as a collar, tie, belt or waistband. If a person vomits place them in the recovery position so that vomit will not reenter the mouth and throat. Rinse mouth. Keep victim warm and quiet. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
Symptoms/effects:	
Acute:	No data available
Delayed:	No data available
Immediate medical attention:	WARNING: It might be hazardous to the person providing aid to give mouth-to-mouth respiration, because the inhaled material is harmful. If breathing has stopped, perform artificial respiration. Use first aid treatment according to the nature of the injury. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.

5. FIRE-FIGHTING MEASURES

Suitable extinguishing media: Dry chemical, CO₂, sand, earth, water spray or regular foam Consult with local fire authorities before attempting large scale fire fighting operations.

Specific hazards arising from the chemical

Hazardous combustion products: These products include: Carbon oxides Nitrogen oxides Halogenated compounds
Other specific hazards: WARNING: Highly toxic HCl gas is produced during combustion.

Special precautions for fire-fighters:

Use water spray or fog; do not use straight streams. Dike fire-control water for later disposal; do not scatter the material. Containers may explode when heated. Move containers from fire area if you can do it without risk.

Special protective equipment for fire-fighters:

Wear positive pressure self-contained breathing apparatus (SCBA). Structural fire fighters' protective clothing provides limited protection in fire situations ONLY; it may not be effective in spill situations. Wear chemical protective clothing which is specifically recommended by the manufacturer. It may provide little or no thermal protection.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions:	Avoid contact with skin, eyes, and clothing. Keep people away from and upwind of spill/leak. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing (Section 8). Warn unnecessary personnel to move away. Stop leak if you can do it without risk. Ensure adequate ventilation. Isolate the hazard area and deny entry to unnecessary and unprotected personnel.
Personal protective equipment:	Safety glasses. Lab coat. Dust respirator. Be sure to use a MSHA/NIOSH approved respirator or equivalent. Wear protective gloves (nitrile).
Emergency procedures:	Prevent dust cloud. In case of a spill and/or a leak, always shut off any sources of ignition, ventilate the area, and exercise caution. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Warn personnel to move away. Prevent entry into sewers, basements or confined areas; dike if needed.

Methods and materials for containment and cleaning up:

ELIMINATE all ignition sources (no smoking, flares, sparks, or flames in immediate area). Stop leak if without risk. Ventilate the area. Absorb with an inert material and put the spilled material in an appropriate waste disposal container. Use clean non-sparking tools to collect absorbed material.

Environmental precautions:

Keep away from living quarters. Prevent further leakage or spillage if safe to do so. Water runoff can cause environmental damage. Prevent entry into sewers, basements or confined areas; dike if needed.

7. HANDLING AND STORAGE

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Precautions for safe handling:	Avoid inhalation of vapor or mist. Do not ingest. Avoid contact with skin and eyes. Good general ventilation should be sufficient to control airborne levels. Keep container dry. Handle and open container with care. Wear suitable protective clothing, gloves and eye/face protection. When using do not eat, drink, or smoke. Keep away from sources of ignition.
Conditions for safe storage:	Keep only in the original container in a cool well-ventilated place. Keep away from incompatibles. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Avoid prolonged storage periods.
Storage incompatibilities:	Store away from oxidizing agents

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Exposure limits: No data available

Appropriate engineering controls:

Good general ventilation should be sufficient to control airborne levels. Ventilation is normally required when handling or using this product. Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substance. Follow safe industrial engineering/laboratory practices when handling any chemical.

Personal protective equipment

Respiratory protection:	Dust respirator. Be sure to use a MSHA/NIOSH approved respirator or equivalent.
Hand protection:	Wear protective gloves.
Eye protection:	Safety glasses.
Skin and body protection:	Lab coat.

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state (20°C):	Solid
Form:	Crystal - Powder
Color:	White - Very pale yellow
Odor:	No data available
Odor threshold:	No data available

Melting point/freezing point:	145°C (293°F)	pH:	No data available
Boiling point/range:	No data available	Vapor pressure:	No data available
Decomposition temperature:	No data available	Vapor density:	No data available
Relative density:	No data available	Dynamic Viscosity:	No data available
Kinematic Viscosity:	No data available		
Partition coefficient: n-octanol/water (log P_{ow})	No data available	Evaporation rate: (Butyl Acetate = 1)	No data available
Flash point:	No data available	Autoignition temperature:	No data available
Flammability (solid, gas):	No data available	Flammability or explosive limits:	
		Lower:	No data available
		Upper:	No data available

Solubility(ies):

10. STABILITY AND REACTIVITY

Reactivity:	Not Available.
Chemical Stability:	Stable under recommended storage conditions. (See Section 7)
Possibility of Hazardous Reactions:	No hazardous reactivity has been reported.
Conditions to avoid:	Avoid excessive heat and light.
Incompatible materials:	Oxidizing agents
Hazardous Decomposition Products:	No data available

11. TOXICOLOGICAL INFORMATION

Acute Toxicity:
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

IARC: No data available

NTP: No data available

OSHA: No data available

Reproductive toxicity:
No data available

Routes of Exposure: Inhalation, Eye contact, Ingestion.

Symptoms related to exposure:
Overexposure may result in serious illness or death.

Potential Health Effects:
No specific information available; skin and eye contact may result in irritation. May be harmful if inhaled or ingested.

Target organ(s): No data available

12. ECOLOGICAL INFORMATION

Ecotoxicity

Fish:	No data available
Crustacea:	No data available
Algae:	No data available

Persistence and degradability:	No data available
Bioaccumulative potential (BCF):	No data available
Mobility in soil:	No data available
Partition coefficient: n-octanol/water (log P_{ow})	No data available
Soil adsorption (K_{oc}):	No data available
Henry's Law: constant (PaM³/mol)	No data available

13. DISPOSAL CONSIDERATIONS

Disposal of product:	Recycle to process if possible. It is the generator's responsibility to comply with Federal, State and Local rules and regulations. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. This section is intended to provide assistance but does not replace these laws, nor does compliance in accordance with this section ensure regulatory compliance according to the law. US EPA guidelines for Identification and Listing of Hazardous Waste are listed in 40 CFR Parts 261. The product should not be allowed to enter the environment, drains, water ways, or the soil.
Disposal of container:	Dispose of as unused product. Do not re-use empty containers.
Other considerations:	Observe all federal, state and local regulations when disposing of the substance.

14. TRANSPORT INFORMATION

DOT (US) Non-hazardous for transportation.

IATA Non-hazardous for transportation.

IMDG Non-hazardous for transportation.

15. REGULATORY INFORMATION**Toxic Substance Control Act (TSCA 8b.):**

This product is NOT on the EPA Toxic Substances Control Act (TSCA) inventory. The following notices are required by 40 CFR 720.36 (C) for those products not on the inventory list:

- (i) These products are supplied solely for use in research and development by or under the supervision of a technically qualified individual as defined in 40 CFR 720.0 et sec.
- (ii) The health risks of these products have not been fully determined. Any information that is or becomes available will be supplied on a SDS sheet.

US Federal Regulations**CERCLA Hazardous substance and Reportable Quantity:**

SARA 313: Not Listed
SARA 302: Not Listed

State Regulations**State Right-to-Know**

Massachusetts Not Listed
New Jersey Not Listed
Pennsylvania Not Listed
California Proposition 65: Not Listed

Other Information**NFPA Rating:**

Health: 2
Flammability: 0
Instability: 0

HMIS Classification:

Health: 2
Flammability: 0
Physical: 0

International Inventories

WHMIS hazard class: D2A: Materials causing other toxic effects. (Very Toxic)

16. OTHER INFORMATION

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TCI chemicals are for research purposes only and are NOT intended for use as drugs, food additives, households, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its affiliates or subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our SDS are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated SDS for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, face mask, fume hood). For proper handling and disposal, always comply with federal, state and local regulations.