



TCI EUROPE N.V.

# SAFETY DATA SHEET

According to 1907/2006/EC, Article 31

Revision number: 1

Revision date: 10/02/2018

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

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

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

**Identified uses:** Reagents.

### 1.3 Details of the supplier of the safety data sheet

**Supplier:**

TCI EUROPE N.V.  
Boerenveldseweg 6  
Haven 1063  
B-2070 Zwijndrecht  
Telephone: +32(0)3 735 07 00  
E-mail: sales-eu@tcichemicals.com

**1.4 Emergency telephone number:** +32(0)70 245 245

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

**Acute toxicity (Oral)** Category 4

### 2.2 Label elements

**Pictograms or hazard symbols**



**Signal word**

**Hazard statements**

**Precautionary statements**

Warning  
H302-Harmful if swallowed.  
P270-Do not eat, drink or smoke when using this product.  
P264-Wash hands and face thoroughly after handling.  
P301+P312+P330-IF SWALLOWED: Call a POISON CENTER or doctor if you feel unwell. Rinse mouth.  
P501-Dispose of contents/container through a waste management company authorized by the local government.

### 2.3 Other hazards

**Results of PBT and vPvB assessment**

**PBT:** Not applicable  
**vPvB:** Not applicable

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

**Components:** 1-(3-Chloropropyl)theobromine  
**Percent:** >97.0%(HPLC)(T)  
**CAS RN:** 74409-52-2  
**Synonyms:** 1-(3-Chloropropyl)-3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione ,  
1-(3-Chloropropyl)-3,7-dimethylxanthine  
**Chemical Formula:** C<sub>10</sub>H<sub>13</sub>ClN<sub>4</sub>O<sub>2</sub>

#### SECTION 4: First aid measures

##### 4.1 Description of first aid measures

|                                    |  |
|------------------------------------|--|
| <b>Inhalation:</b>                 | Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical advice/attention if you feel unwell.  |
| <b>Skin contact:</b>               | Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower. If skin irritation or rash occurs: Get medical advice/attention.                          |
| <b>Eye contact:</b>                | Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention. |
| <b>Ingestion:</b>                  | Call a POISON CENTER or doctor/physician if you feel unwell. Rinse mouth.  |
| <b>Protection of first-aiders:</b> | A rescuer should wear personal protective equipment, such as rubber gloves and air-tight goggles.  |

##### 4.2 Most important symptoms and effects, both acute and delayed

No data available

##### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

#### SECTION 5: Firefighting measures

##### 5.1 Extinguishing media

**Suitable extinguishing media:** Dry chemical, foam, water spray, carbon dioxide.

##### 5.2 Special hazards arising from the substance or mixture

Take care as it may decompose upon combustion or in high temperatures to generate poisonous fume. Carbon dioxide, Carbon monoxide, Nitrogen oxides (NOx), Hydrogen chloride

##### 5.3 Advice for firefighters

Fire-extinguishing work is done from the windward and the suitable fire-extinguishing method according to the surrounding situation is used. Uninvolved persons should evacuate to a safe place. In case of fire in the surroundings: Remove movable containers if safe to do so. When extinguishing fire, be sure to wear personal protective equipment

#### SECTION 6: Accidental release measures

##### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Keep people away from and upwind of spill/leak. Entry to non-involved personnel should be controlled around the leakage area by roping off, etc

##### 6.2 Environmental precautions

Prevent product from entering drains

##### 6.3 Methods and materials for containment and cleaning up

Sweep dust to collect it into an airtight container, taking care not to disperse it. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

##### 6.4 Reference to other sections

For disposal see section 13.

#### SECTION 7: Handling and storage

##### 7.1 Precautions for safe handling

Handling is performed in a well ventilated place. Wear suitable protective equipment. Prevent dispersion of dust. Wash hands and face thoroughly after handling. Use a local exhaust if dust or aerosol will be generated. Avoid contact with skin, eyes and clothing.

##### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed. Store in a cool and dark place. Store away from incompatible materials such as oxidizing agents.

##### 7.3 Specific end use(s)

No further relevant information available.

#### SECTION 8: Exposure controls/personal protection

##### 8.1 Control parameters

No data available

##### 8.2 Exposure controls

Install a closed system or local exhaust as possible so that workers should not be exposed directly. Also install safety shower and eye bath.

##### **Respiratory protection:**

Dust respirator. Follow local and national regulations.

##### **Hand protection:**

Protective gloves.

##### **Eye protection:**

Safety glasses. A face-shield, if the situation requires.

##### **Skin and body protection:**

Protective clothing. Protective boots, if the situation requires.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

|                                    |                          |
|------------------------------------|--------------------------|
| Physical state (20°C):             | Solid                    |
| Form:                              | Crystal - Powder         |
| Colour:                            | White - Very pale yellow |
| Odour:                             | No data available        |
| pH:                                | No data available        |
| Melting point/freezing point:      | 145°C                    |
| Boiling point/range:               | No data available        |
| Flash point:                       | No data available        |
| Evaporation rate(Butyl Acetate=1): | No data available        |
| Flammability(solid, gas):          | No data available        |
| Flammability or explosive limits:  |                          |
| Lower:                             | No data available        |
| Upper:                             | No data available        |
| Vapour pressure:                   | No data available.       |
| Vapour density:                    | No data available        |
| Relative density:                  | No data available        |
| Solubility(ies):                   |                          |
| [Water]                            | No data available        |
| [Other solvents]                   | No data available        |
| Partition coefficient:             | No data available        |
| n-octanol/water:                   |                          |
| Autoignition temperature:          | No data available        |
| Decomposition temperature:         | No data available        |
| Dynamic Viscosity:                 | No data available        |
| Kinematic viscosity:               | No data available        |

9.2 Other safety information No data available

## SECTION 10: Stability and reactivity

10.1 Reactivity No data available

10.2 Chemical stability Stable under proper conditions.

10.3 Possibility of hazardous reactions No special reactivity has been reported.

10.4 Conditions to avoid No data available

10.5 Incompatible materials Oxidizing agents

10.6 Hazardous decomposition products Carbon dioxide, Carbon monoxide, Nitrogen oxides (NOx), Hydrogen chloride

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

|                                    |                   |
|------------------------------------|-------------------|
| 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:                   |                   |
| IARC =                             | No data available |
| NTP =                              | No data available |
| Reproductive toxicity:             | No data available |
| STOT-single exposure:              | No data available |
| STOT-repeated exposure:            | No data available |
| Aspiration hazard:                 | No data available |

## SECTION 12: Ecological information

|  |                   |
|--|-------------------|
| <b>12.1 Toxicity</b>                           |                   |
| <b>Fish:</b>                                   | No data available |
| <b>Crustacea:</b>                              | No data available |
| <b>Algae:</b>                                  | No data available |
| <b>12.2 Persistence and degradability</b>      | No data available |
| <b>12.3 Bioaccumulative potential</b>          | No data available |
| <b>12.4 Mobility in soil</b>                   |                   |
| <b>Log Pow:</b>                                | No data available |
| <b>Soil adsorption (Koc):</b>                  | No data available |
| <b>Henry's Law (PaM<sup>3</sup>/mol):</b>      | No data available |
| <b>12.5 Results of PBT and vPvB assessment</b> |                   |
| <b>PBT:</b>                                    | Not applicable    |
| <b>vPvB:</b>                                   | Not applicable    |
| <b>12.6 Other adverse effects</b>              | No data available |

## SECTION 13: Disposal considerations

|   |  |
|---|--|
| <b>13.1 Waste treatment methods</b>   |  |
| Recycle to process, if possible. Consult your local regional authorities. 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. Observe all federal, state and local regulations when disposing of the substance. |  |

## SECTION 14: Transport information

|  |  |
|--|--|
| <b>14.1 UN number</b>                    | Not listed   |
| <b>14.2 UN proper shipping name</b>      |  |
| <b>ADR/RID</b>                           | Not listed   |
| <b>IMDG/IMO</b>                          | Not listed   |
| <b>ICAO/IATA</b>                         | Not listed   |
| <b>14.3 Transport hazard class(es)</b>   |  |
| <b>ADR/RID</b>                           | Does not correspond to the classification standard of the United Nations |
| <b>IMDG/IMO</b>                          | Does not correspond to the classification standard of the United Nations |
| <b>ICAO/IATA</b>                         | Does not correspond to the classification standard of the United Nations |
| <b>14.4 Packaging group</b>              |  |
| <b>ADR/RID</b>                           | -  |
| <b>IMDG/IMO</b>                          | -  |
| <b>ICAO/IATA</b>                         | -  |
| <b>14.5 Environmental hazards</b>        |  |
| <b>Marine pollutant</b>                  | -  |
| <b>14.6 Special precautions for user</b> | No data available  |

## SECTION 15: Regulatory information

|  |  |
|--|--|
| <b>15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture</b> |  |
| <b>Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No.1907/2006</b>          | Not listed   |
| <b>15.2 Chemical safety assessment</b>   | A chemical safety assessment has not been carried out. |

**SECTION 16: Other information**

**Prepared by:** TCI EUROPE N.V.  
**Issue date:** 10/02/2018

This SDS was prepared sincerely on the basis of the information we could obtain, however, any warranty shall not be given regarding the data contained and the assessment of hazards and toxicity. Prior to use, please investigate not only the hazards and toxicity information but also the laws and regulations of the organization, area and country where the products are to be used, which shall be given the first priority. The products are supposed to be used promptly after purchase in consideration of safety. Some new information or amendments may be added afterwards. If the products are to be used far behind the expected time of use or you have any questions, please feel free to contact us. The stated cautions are for normal handling only. In case of special handling, sufficient care should be taken, in addition to the safety measures suitable for the situation. All chemical products should be treated with the recognition of "having unknown hazards and toxicity", which differ greatly depending on the conditions and handling when in use and/or the conditions and duration of storage. The products must be handled only by those who are familiar with specialized knowledge and have experience or under the guidance of those specialists throughout use from opening to storage and disposal. Safe usage conditions shall be set up on each user's own responsibility.

**End of Safety Data Sheet**