



# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

## SECTION 1: Identification

### 1.1 GHS Product identifier

Product name 1-(3-Chloropropyl)theobromine

### 1.2 Other means of identification

Product number -  
Other names 1-(3-chloropropyl)-3,7-dimethylpurine-2,6-dione;

### 1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research use.  
Uses advised against no data available

### 1.4 Supplier's details

Company Shanghai Yien Chemical Technology Co., Ltd  
Address Building 6, 28 Yingong Road, Fengxian District, Shanghai  
Chemical Industry Zone, Shanghai, 201400, China  
Telephone +86-400-133-2688

### 1.5 Emergency phone number

Emergency phone number +86-400-133-2688  
Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

## SECTION 2: Hazard identification

### 2.1 Classification of the substance or mixture

Acute toxicity - Category 4, Oral

### 2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word Warning  
Hazard statement(s) H302 Harmful if swallowed  
Precautionary statement(s)  
Prevention P264 Wash ... thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
Response P301+P317 IF SWALLOWED: Get medical help.  
P330 Rinse mouth.

<b>Storage</b>	none
<b>Disposal</b>	P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

## 2.3 Other hazards which do not result in classification

no data available

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
1-(3-Chloropropyl)theobromine	1-(3-Chloropropyl)theobromine	74409-52-2	-	100%

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## SECTION 4: First-aid measures

### 4.1 Description of necessary first-aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

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

no data available

### 4.3 Indication of immediate medical attention and special treatment needed, if necessary

no data available

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## SECTION 5: Fire-fighting measures

### 5.1 Suitable extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

### 5.2 Specific hazards arising from the chemical

no data available

### 5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

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## SECTION 6: Accidental release measures

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

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure

adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

## **6.2 Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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# **SECTION 7: Handling and storage**

## **7.1 Precautions for safe handling**

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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

## **8.1 Control parameters**

### **Occupational Exposure limit values**

no data available

### **Biological limit values**

no data available

## **8.2 Appropriate engineering controls**

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

## **8.3 Individual protection measures, such as personal protective equipment (PPE)**

### **Eye/face protection**

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### **Skin protection**

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### **Respiratory protection**

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### **Thermal hazards**

no data available

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# **SECTION 9: Physical and chemical properties and safety characteristics**

## **Physical state**

no data available

<b>Colour</b>	no data available
<b>Odour</b>	no data available
<b>Melting point/freezing point</b>	104°C(lit.)
<b>Boiling point or initial boiling point and boiling range</b>	116°C/16mmHg(lit.)
<b>Flammability</b>	no data available
<b>Lower and upper explosion limit/flammability limit</b>	no data available
<b>Flash point</b>	101°C(lit.)
<b>Auto-ignition temperature</b>	no data available
<b>Decomposition temperature</b>	no data available
<b>pH</b>	no data available
<b>Kinematic viscosity</b>	no data available
<b>Solubility</b>	no data available
<b>Partition coefficient n-octanol/water</b>	no data available
<b>Vapour pressure</b>	no data available
<b>Density and/or relative density</b>	1.46g/cm <sup>3</sup>
<b>Relative vapour density</b>	no data available
<b>Particle characteristics</b>	no data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

no data available

### 10.3 Possibility of hazardous reactions

no data available

### 10.4 Conditions to avoid

no data available

### 10.5 Incompatible materials

no data available

### 10.6 Hazardous decomposition products

no data available

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: 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

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

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**SECTION 12: Ecological information****12.1 Toxicity**

- Toxicity to fish: no data available
- Toxicity to daphnia and other aquatic invertebrates: no data available
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

**12.2 Persistence and degradability**

no data available

**12.3 Bioaccumulative potential**

no data available

**12.4 Mobility in soil**

no data available

**12.5 Other adverse effects**

no data available

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**SECTION 13: Disposal considerations****13.1 Disposal methods****Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

**Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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**SECTION 14: Transport information****14.1 UN Number**

ADR/RID: UN3267 (For reference only, please check.)

IMDG: UN3267 (For reference only, please check.)

IATA: UN3267 (For reference only, please check.)

## 14.2 UN Proper Shipping Name

ADR/RID: CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S. (For reference only, please check.)

IMDG: CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S. (For reference only, please check.)

IATA: CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S. (For reference only, please check.)

## 14.3 Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.)

IMDG: 8 (For reference only, please check.)

IATA: 8 (For reference only, please check.)

## 14.4 Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

## 14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

## 14.6 Special precautions for user

no data available

## 14.7 Transport in bulk according to IMO instruments

no data available

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# SECTION 15: Regulatory information

## 15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
1-(3-Chloropropyl)theobromine	1-(3-Chloropropyl)theobromine	74409-52-2	-
European Inventory of Existing Commercial Chemical Substances (EINECS)			Not Listed.
EC Inventory			Not Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Not Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
New Zealand Inventory of Chemicals (NZIoC)			Not Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Not Listed.
Vietnam National Chemical Inventory			Not Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Not Listed.
Korea Existing Chemicals List (KECL)			Not Listed.

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# SECTION 16: Other information

### Information on revision

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### Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

## References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisys.com](mailto:sds@xixisys.com)**

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