

# Safety Data Sheet

acc. to OSHA HCS

Printing date 09/15/2020

Revision date 09/15/2020

## 1 Identification

- **Product identifier**
- **Trade name:** Theobromine-d6
- **Article number:** 9003565
- **CAS Number:**  
117490-40-1
- **EC number:**  
694-176-1
- **Application of the substance / the mixture** For research use only - not for human or veterinary use.
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**  
Cayman Chemical Co.  
1180 E. Ellsworth Rd.  
Ann Arbor, MI 48108  
USA
- **Information department:** Product safety department
- **Emergency telephone number:**  
During normal opening times: +1 (734) 971-3335  
US/CANADA: 800-424-9300  
Outside US/CANADA: 703-741-5970

## 2 Hazard(s) identification

- **Classification of the substance or mixture**



Acute Tox. 4 H302 Harmful if swallowed.

- **Label elements**
- **GHS label elements**  
The substance is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



- **Signal word** Warning
- **Hazard statements**  
Harmful if swallowed.
- **Precautionary statements**  
Wash thoroughly after handling.  
Do not eat, drink or smoke when using this product.  
If swallowed: Call a poison center/doctor if you feel unwell.  
Rinse mouth.  
Dispose of contents/container in accordance with local/regional/national/international regulations.

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- **Classification system:**
- **NFPA ratings (scale 0 - 4)**



Health = 2  
Fire = 0  
Reactivity = 0

- **HMIS-ratings (scale 0 - 4)**



Health = 2  
Fire = 0  
Reactivity = 0

- **Other hazards**
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.

## 3 Composition/information on ingredients

- **Chemical characterization: Substances**
- **CAS No. Description**  
117490-40-1 Theobromine-d6
- **Identification number(s)**
- **EC number:** 694-176-1

## 4 First-aid measures

- **Description of first aid measures**
- **General information:**  
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
- **After inhalation:** Supply fresh air; consult doctor in case of complaints.
- **After skin contact:** Generally the product does not irritate the skin.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **After swallowing:** Immediately call a doctor.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed**  
May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects.  
No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**  
No further relevant information available.

## 5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**  
Use fire fighting measures that suit the environment.  
A solid water stream may be inefficient.
- **Special hazards arising from the substance or mixture** No further relevant information available.

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- **Advice for firefighters**
- **Protective equipment:** No special measures required.

## 6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures** Not required.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:** Pick up mechanically.
- **Reference to other sections**  
See Section 7 for information on safe handling.  
See Section 8 for information on personal protection equipment.  
See Section 13 for disposal information.
- **Protective Action Criteria for Chemicals**
- **PAC-1:** Substance is not listed.
- **PAC-2:** Substance is not listed.
- **PAC-3:** Substance is not listed.

## 7 Handling and storage

- **Handling:**
- **Precautions for safe handling**  
No special precautions are necessary if used correctly.  
Avoid breathing dust/fume/gas/mist/vapours/spray.  
Avoid prolonged or repeated exposure.  
Keep away from sources of ignition.  
Take precautionary measures against static discharge.re.
- **Information about protection against explosions and fires:** No special measures required.
- **Conditions for safe storage, including any incompatibilities**  
Keep container tightly closed.  
Store in accordance with information listed on the product insert.
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** None.
- **Specific end use(s)** No further relevant information available.

## 8 Exposure controls/personal protection

- **Additional information about design of technical systems:** No further data; see item 7.
- **Control parameters**
- **Components with limit values that require monitoring at the workplace:**  
The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.  
The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit.  
At this time, the remaining constituent has no known exposure limits.  
At this time, the other constituents have no known exposure limits.
- **Additional information:** The lists that were valid during the creation were used as basis.

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- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:** Wash hands before breaks and at the end of work.
- **Breathing equipment:** Not required.
- **Protection of hands:**  
The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.  
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.  
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
- **Material of gloves**  
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material**  
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
- **Eye protection:** Not required.

## 9 Physical and chemical properties

### · Information on basic physical and chemical properties

#### · General Information

#### · Appearance:

- |                             |                 |
|-----------------------------|-----------------|
| · <b>Form:</b>              | Solid           |
| · <b>Color:</b>             | Not determined. |
| · <b>Odor:</b>              | Characteristic  |
| · <b>Structural Formula</b> | C7H2D6N4O2      |
| · <b>Molecular Weight</b>   | 186.2 g/mol     |
| · <b>Odor threshold:</b>    | Not determined. |

- |                    |                 |
|--------------------|-----------------|
| · <b>pH-value:</b> | Not applicable. |
|--------------------|-----------------|

#### · Change in condition

- |                                       |               |
|---------------------------------------|---------------|
| · <b>Melting point/Melting range:</b> | Undetermined. |
| · <b>Boiling point/Boiling range:</b> | Undetermined. |

- |                       |                 |
|-----------------------|-----------------|
| · <b>Flash point:</b> | Not applicable. |
|-----------------------|-----------------|

- |   |                           |
|---|---------------------------|
| · <b>Flammability (solid, gaseous):</b> | Product is not flammable. |
|---|---------------------------|

- |                                     |                 |
|-------------------------------------|-----------------|
| · <b>Decomposition temperature:</b> | Not determined. |
|-------------------------------------|-----------------|

- |                         |                 |
|-------------------------|-----------------|
| · <b>Auto igniting:</b> | Not determined. |
|-------------------------|-----------------|

- |                               |   |
|-------------------------------|---|
| · <b>Danger of explosion:</b> | Product does not present an explosion hazard. |
|-------------------------------|---|

#### · Explosion limits:

- |                 |                 |
|-----------------|-----------------|
| · <b>Lower:</b> | Not determined. |
| · <b>Upper:</b> | Not determined. |

- |                          |                 |
|--------------------------|-----------------|
| · <b>Vapor pressure:</b> | Not applicable. |
|--------------------------|-----------------|

- |                           |                 |
|---------------------------|-----------------|
| · <b>Density:</b>         | Not determined. |
| · <b>Relative density</b> | Not determined. |
| · <b>Vapor density</b>    | Not applicable. |
| · <b>Evaporation rate</b> | Not applicable. |

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- |   |  |
|---|--|
| · <b>Solubility in / Miscibility with Water:</b>  | Not determined.                            |
| · <b>Partition coefficient (n-octanol/water):</b> | Not determined.                            |
| · <b>Viscosity:</b>                               |  |
| <b>Dynamic:</b>                                   | Not applicable.                            |
| <b>Kinematic:</b>                                 | Not applicable.                            |
| <b>SOLUBILITY</b>                                 | DMSO                                       |
| · <b>Other information</b>                        | No further relevant information available. |

## 10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:**  
No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** strong oxidizing agents
- **Hazardous decomposition products:** carbon oxides, nitrogen oxides

## 11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**
- **Primary irritant effect:**
- **on the skin:** No irritant effect.
- **on the eye:** No irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional toxicological information:**
- **Carcinogenic categories**
- **IARC (International Agency for Research on Cancer)** Substance is not listed.
- **NTP (National Toxicology Program)** Substance is not listed.
- **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.

## 12 Ecological information

- **Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **Persistence and degradability** No further relevant information available.
- **Behavior in environmental systems:**
- **Bioaccumulative potential** No further relevant information available.
- **Mobility in soil** No further relevant information available.
- **Additional ecological information:**
- **General notes:**  
Water hazard class 1 (Self-assessment): slightly hazardous for water  
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

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- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Other adverse effects** No further relevant information available.

### 13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**  
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

### 14 Transport information

· <b>UN-Number</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>UN proper shipping name</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>Transport hazard class(es)</b>	
· <b>DOT, ADN, IMDG, IATA</b>	
· <b>Class</b>	not regulated
· <b>Packing group</b>	
· <b>DOT, IMDG, IATA</b>	not regulated
· <b>Environmental hazards:</b>	Not applicable.
· <b>Special precautions for user</b>	Not applicable.
· <b>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	Not applicable.
· <b>UN "Model Regulation":</b>	not regulated

### 15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**
- **Sara**
- **Section 355 (extremely hazardous substances):** Substance is not listed.
- **Section 313 (Specific toxic chemical listings):** Substance is not listed.
- **TSCA (Toxic Substances Control Act):** Substance is not listed.
- **Hazardous Air Pollutants** Substance is not listed.
- **Proposition 65**
- **Chemicals known to cause cancer:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
- **Chemicals known to cause developmental toxicity:** Substance is not listed.

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- **Carcinogenic categories**
- **EPA (Environmental Protection Agency)** Substance is not listed.
- **TLV (Threshold Limit Value established by ACGIH)** Substance is not listed.
- **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
- **GHS label elements**  
The substance is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



GHS07

- **Signal word** Warning
- **Hazard statements**  
Harmful if swallowed.
- **Precautionary statements**  
Wash thoroughly after handling.  
Do not eat, drink or smoke when using this product.  
If swallowed: Call a poison center/doctor if you feel unwell.  
Rinse mouth.  
Dispose of contents/container in accordance with local/regional/national/international regulations.
- **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

## 16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- **Department issuing SDS:** Environment protection department.
- **Contact:** -
- **Date of preparation / last revision** 09/15/2020 / -
- **Abbreviations and acronyms:**  
IMDG: International Maritime Code for Dangerous Goods  
DOT: US Department of Transportation  
IATA: International Air Transport Association  
ACGIH: American Conference of Governmental Industrial Hygienists  
EINECS: European Inventory of Existing Commercial Chemical Substances  
CAS: Chemical Abstracts Service (division of the American Chemical Society)  
NFPA: National Fire Protection Association (USA)  
HMIS: Hazardous Materials Identification System (USA)  
PBT: Persistent, Bioaccumulative and Toxic  
vPvB: very Persistent and very Bioaccumulative  
NIOSH: National Institute for Occupational Safety  
OSHA: Occupational Safety & Health  
TLV: Threshold Limit Value  
PEL: Permissible Exposure Limit  
REL: Recommended Exposure Limit  
Acute Tox. 4: Acute toxicity – Category 4

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