1 Identification

Product identifier

Product name: Theobromine

Stock number: A11861, L04360

CAS Number: 83-67-0

EC number: 201-494-2

Relevant identified uses of the substance or mixture and uses advised against.

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)

GHS06 Skull and crossbones

Acute Tox. 3 H301 Toxic if swallowed.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms

GHS06

Signal word Danger

Hazard statements

H301 Toxic if swallowed.

Precautionary statements

P264 Wash thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/…

P321 Specific treatment (see on this label).

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

D1B - Toxic material causing immediate and serious toxic effects

Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH = 2

FLAMMABILITY = 1

REACTIVITY = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description: 83-67-0 Theobromine

Identification number(s):

EC number: 201-494-2

4 First-aid measures

Description of first aid measures

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly. Seek immediate medical advice.

After eye contact

Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Seek medical treatment.

(Contd. on page 2)
5 Fire-fighting measures

Extinguishing media
Suitable extinguishing agents: Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Nitrogen oxides (NOx)

Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.

Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.

Methods and material for containment and cleaning up: Dispose of contaminated material as waste according to section 13.

Prevention of secondary hazards: No special measures required.

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.

7 Handling and storage

Handling
Precautions for safe handling
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.

Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities

Storage
Requirements to be met by storerooms and receptacles: No special requirements.

Information about storage in one common storage facility: Store away from oxidizing agents.

Further information about storage conditions:
Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.

Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters
Components with limit values that require monitoring at the workplace: Not required.

Additional information: No data

Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Maintain an ergonomically appropriate working environment.
Breathing equipment: Use suitable respirator when high concentrations are present.

Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition. The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

Eye protection: Safety glasses

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties
General Information
Appearance:
Form: Powder
Color: White
Odor: Not determined
Odor threshold: Not determined.

pH-value: Not applicable.

Change in condition
Melting point/Melting range: 345-350 °C (653-662 °F)
Boiling point/Boiling range: Not determined
Sublimation temperature / start: Not determined

Flash point: Not applicable

Flammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined

Auto igniting: Not determined.

Danger of explosion: Product does not present an explosion hazard.
Explosion limits:

<table>
<thead>
<tr>
<th>Lower:</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Upper:</td>
<td>Not determined</td>
</tr>
</tbody>
</table>

Vapor pressure:

- Not applicable.

Density:

- Not determined.

Relative density:

- Not determined.

Vapor density:

- Not applicable.

Evaporation rate:

- Not applicable.

Solubility in / Miscibility with:

- Water: Not determined

Partition coefficient (n-octanol/water):

- Not determined.

Viscosity:

- Dynamic: Not applicable.
- Kinematic: Not applicable.

Other information:

- No further relevant information available.

10 Stability and reactivity

Reactivity: No information known.

Chemical stability: Stable under recommended storage conditions.

Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.

Possibility of hazardous reactions: No dangerous reactions known.

Conditions to avoid: No further relevant information available.

Incompatible materials: Oxidizing agents.

Hazardous decomposition products:

- Carbon monoxide and carbon dioxide
- Nitrogen oxides

11 Toxicological information

Information on toxicological effects

Acute toxicity: Harmful if swallowed.

LD/LC50 values that are relevant for classification: No data.

Skin irritation or corrosion: Irritant to skin and mucous membranes.

Eye irritation or corrosion: Irritating effect.

Sensitization: No sensitizing effects known.

Germ cell mutagenicity: No effects known.

Carcinogenicity: IARC-3: Not classifiable as to carcinogenicity to humans.

Reproductive toxicity: No effects known.

Specific target organ system toxicity - repeated exposure: No effects known.

Specific target organ system toxicity - single exposure: No effects known.

Aspiration hazard: No effects known.

Other information (about experimental toxicology):

- Reproductive effects have been observed on tests with laboratory animals.
- Mutagenic effects have been observed on tests with bacteria.
- Mutagenic effects have been observed on tests with human lymphocytes.
- Mutagenic effects have been observed on tests with human and/or animal DNA cells.
- Mutagenic effects have been observed on tests with laboratory animals.

Subacute to chronic toxicity:

- The Registry of Toxic Effects of Chemical Substances (RTECS) reports the following effects in laboratory animals:
  - Behavioral - changes in motor activity (specific assay).
  - Behavioral - convulsions or effect on seizure threshold.
  - Behavioral - food intake (animal).
  - Cardiac - other changes.
  - Gastrointestinal - nausea or vomiting.
  - Blood - changes in serum composition (e.g. TP, bilirubin, cholesterol).
  - Biochemical - Enzyme inhibition, induction, or change in blood or tissue levels - other transferases.
  - Endocrine - changes in thymus weight.
  - Endocrine - other changes.
  - Related to Chronic Data - changes in testicular weight.
  - Related to Chronic Data - death.
  - Nutritional and Gross Metabolic - weight loss or decreased weight gain.
  - Reproductive - Paternal Effects - testis, epididymis, sperm duct.
  - Reproductive - Fertility - male fertility index (e.g. # males impregnating females per # males exposed to fertile nonpregnant females)
  - Reproductive - Effects on Newborn - live birth index (measured after birth)
  - Reproductive - Effects on Newborn - growth statistics (e.g. %, reduced weight gain).
  - Reproductive - Effects on Embryo or Fetus - fetotoxicity (except death, e.g., stunted fetus).
  - Reproductive - Specific Developmental Abnormalities - craniofacial (including nose and tongue).
  - Reproductive - Specific Developmental Abnormalities - musculoskeletal system.
  - Reproductive - Specific Developmental Abnormalities - other developmental abnormal.
  - Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity

Aquatic toxicity: No further relevant information available.

Persistence and degradability: No further relevant information available.

Bioaccumulative potential: No further relevant information available.

Mobility in soil: No further relevant information available.

Additional ecological information:

- General notes: Do not allow product to reach ground water, water course or sewage system.
  
- Do not allow material to be released to the environment without proper governmental permits.
  
- Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.

Avoid transfer into the environment.

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: Consult state, local or national regulations to ensure proper disposal.
14 Transport information
Not a hazardous material for transportation.

<table>
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<th>UN-Number</th>
<th>DOT, IMDG, IATA</th>
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<td>Transport hazard class(es)</td>
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<td>Packing group</td>
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<td>Environmental hazards:</td>
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<tr>
<td>Special precautions for user</td>
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</tr>
<tr>
<td>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</td>
<td></td>
<td>Not applicable.</td>
</tr>
</tbody>
</table>

15 Regulatory information
Safety, health and environmental regulations/legislation specific for the substance or mixture

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms

GHS06

Signal word Danger
Hazard statements
H301 Toxic if swallowed.

Precautionary statements
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P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

National regulations
All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.
SARA Section 313 (specific toxic chemical listings) Substance is not listed.
California Proposition 65
Prop 65 - Chemicals known to cause cancer Substance is not listed.
Prop 65 - Developmental toxicity, female Substance is not listed.
Prop 65 - Developmental toxicity, male Substance is not listed.
Information about limitation of use: For use only by technically qualified individuals.

Other regulations, limitations and prohibitive regulations
Although this chemical may sometimes be used as a food or drug or cosmetic, our products are not approved or suitable for such use or for human consumption.

Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.
Substance is not listed.
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information
Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department
Date of preparation / last revision 11/23/2015 / -
Abbreviations and acronyms:
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)