1 Identification of substance:

Product details:

Product name: Caffeine
Stock number: 39214

Manufacturer/Supplier:
Alfa Aesar, A Johnson Matthey Company
Johnson Matthey Catalog Company, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Emergency Phone: (978) 521-6300
CHEMTREC: (800) 424-9300
Web Site: www.alfa.com

Information Department: Health, Safety and Environmental Department
Emergency information:
During normal hours the Health, Safety and Environmental Department. After normal hours call Chemtrec at (800) 424-9300.

2 Composition/Data on components:

Chemical characterization:
Description: (CAS#)
1,3,7-Trimethylxanthine (CAS# 58-08-2): 100%

Identification number(s):
EINECS Number: 200-362-1
Index number: 613-086-00-5

3 Hazards identification

Hazard description:

Xn Harmful

Classification system

HMIS ratings (scale 0-4)
(Hazardous Materials Identification System)

HEALTH 2
FIRE 1
REACTIVITY 1

Health (acute effects) = 2
Flammability = 1
Reactivity = 1

GHS label elements

Warning

3.1/4 - Harmful if swallowed.

Prevention:
Wash thoroughly after handling.
Do not eat, drink or smoke when using this product.

Response:
IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
Rinse mouth.

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

4 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.

(Contd. on page 2)
5 Fire fighting measures

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

Special hazards caused by the material, its products of combustion or resulting gases:
In case of fire, the following can be released:
Nitrogen oxides (NOx)
Carbon monoxide and carbon dioxide

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

6 Accidental release measures

Person-related safety precautions:
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation

Measures for environmental protection:
Do not allow material to be released to the environment without proper governmental permits.

Measures for cleaning/collecting:
Dispose contaminated material as waste according to item 13.

Additional information:
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
Information 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 special measures required.

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

Information about storage in one common storage facility:
Do not store together with acids.
Store away from strong bases.
Store away from oxidizing agents.

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

8 Exposure controls and 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.

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

Additional information: No data

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.

Breathing equipment: Use suitable respirator when high concentrations are present.

Protection of hands: Impervious gloves

Eye protection: Safety glasses

Body protection: Protective work clothing.
9 Physical and chemical properties:

General Information

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Form</td>
<td>Powder</td>
</tr>
<tr>
<td>Color</td>
<td>White</td>
</tr>
<tr>
<td>Odor</td>
<td>Odorless</td>
</tr>
<tr>
<td>Melting point/Melting range</td>
<td>234-237°C (453-459°F)</td>
</tr>
<tr>
<td>Boiling point/Boiling range</td>
<td>Not determined</td>
</tr>
<tr>
<td>Sublimation temperature / start</td>
<td>Not determined</td>
</tr>
<tr>
<td>Flash point</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Ignition temperature</td>
<td>Not determined</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>Not determined</td>
</tr>
<tr>
<td>Danger of explosion</td>
<td>Product does not present an explosion hazard.</td>
</tr>
</tbody>
</table>

10 Stability and reactivity

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

Materials to be avoided:

- Acids
- Bases
- Oxidizing agents

Dangerous reactions: No dangerous reactions known.

Dangerous products of decomposition:

- Nitrogen oxides
- Carbon monoxide and carbon dioxide

11 Toxicological information

Acute toxicity:

<table>
<thead>
<tr>
<th>Route</th>
<th>LD50</th>
<th>LDLo</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral</td>
<td>316 mg/kg (bird-wild bird species)</td>
<td>100 mg/kg (cat)</td>
</tr>
<tr>
<td></td>
<td>140 mg/kg (dog)</td>
<td>320 mg/kg (child)</td>
</tr>
<tr>
<td></td>
<td>230 mg/kg (guinea pig)</td>
<td>192 mg/kg (human)</td>
</tr>
<tr>
<td></td>
<td>230 mg/kg (ham)</td>
<td>127 mg/kg (mouse)</td>
</tr>
<tr>
<td></td>
<td>192 mg/kg (rat)</td>
<td>192 mg/kg (human)</td>
</tr>
<tr>
<td></td>
<td>224 mg/kg (rabbit)</td>
<td>1 gm/kg (wmn)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>400 mg/kg (wmn)</td>
</tr>
</tbody>
</table>

Primary irritant effect:

- on the skin: Irritant to skin and mucous membranes.
- on the eye: Irritating effect.

Sensitization: No sensitizing effects known.

Other information (about experimental toxicology):

- Mutagenic effects have been observed on tests with laboratory animals.
- Mutagenic effects have been observed on tests with insects.
- Mutagenic effects have been observed with human leukocyte.
- Mutagenic effects have been observed with human fibroblast.
- Mutagenic effects have been observed on tests with bacteria.
- Tumorigenic effects have been observed on tests with laboratory animals.
- Reproductive effects have been observed on tests with laboratory animals.
**Material Safety Data Sheet**

**Product name: Caffeine**

**Subacute to chronic toxicity:**

Human systemic effects by ingestion, intravenous and intramuscular routes include: convulsions, muscle spasms, tremors, poor muscle coordination, somnolence, nausea or vomiting, and blood pressure increase.

**Subacute to chronic toxicity:**

The Registry of Toxic Effects of Chemical Substances (RTECS) reports the following effects in laboratory animals:

- Behavioral - convulsions or effect on seizure threshold.
- Behavioral - muscle contraction or spasticity.
- Behavioral - hallucinations, distorted perceptions.
- Behavioral - somnolence (general depressed activity).
- Behavioral - ataxia.
- Behavioral - tremor.
- Behavioral - withdrawal.
- Behavioral - toxic psychosis.
- Behavioral - food intake (animal).
- Behavioral - changes in motor activity (specific assay).
- Behavioral - stiffness.
- Behavioral - aggression.

Blood - hemorrhage.

Blood - changes in cell count (unspecified).

Brain and Coverings - other degenerative changes.

Cardiac - other changes.
Cardiac - change in rate.
Cardiac - pulse rate increase, without fall in BP.

Endocrine - changes in pituitary weight.
Endocrine - changes in adrenal weight.
Endocrine - changes in thymus weight.

Gastrointestinal - nausea or vomiting.
Gastrointestinal - hypermotility, diarrhea.
Gastrointestinal - changes in structure or function of salivary glands.
Gastrointestinal - colon tumors.

Kidney, Ureter, Bladder - changes in tubules (including acute renal failure, acute tubular necrosis).

Kidney, Ureter, Bladder - interstitial nephritis.
Kidney, Ureter, Bladder - changes in kidney weight.

Kidney, Ureter, Bladder - structural or functional changes in ureter.
Liver - changes in liver weight.

Lungs, Thorax, or Respiration - cyanosis.
Lungs, Thorax, or Respiration - acute pulmonary edema.
Lungs, Thorax, or Respiration - dyspnea.

Lungs, Thorax, or Respiration - respiratory depression

Kidney, Ureter, Bladder - urine volume increased.

Musculoskeletal - tumors.
Nutritional and Gross Metabolic - weight loss or decreased weight gain.

Related to Chronic Data - changes in testicular weight.
Reproductive - Paternal Effects - spermatogenesis (including genetic material, sperm morphology, motility, and count).
Reproductive - Paternal Effects - testes, epididymis, sperm duct.
Reproductive - Paternal Effects - prostate, seminal vesicle, Cowper’s gland, accessory glands.
Reproductive - Specific Developmental Abnormalities - craniofacial (including nose and tongue).

Reproductive - Specific Developmental Abnormalities - musculoskeletal system.
Reproductive - Effects on Newborn - stillbirth.
Reproductive - Fertility - abortion.
Reproductive - Effects on Newborn - biochemical and metabolic.
Reproductive - Effects on Newborn - other postnatal measures or effects.
Reproductive - Effects on Newborn - behavioral.

Reproductive - Effects on Newborn - physical.
Reproductive - Effects on Embryo or Fetus - extra-embryonic structures (e.g., placenta, umbilical cord).
Reproductive - Effects on Embryo or Fetus - fetotoxicity (except death, e.g., stunted fetus).

Reproductive - Specific Developmental Abnormalities - blood and lymphatic systems (including spleen and marrow).
Reproductive - Specific Developmental Abnormalities - homeostasis.
Reproductive - Fertility - female fertility index (e.g. # females pregnant per # sperm positive females; # females pregnant per # females mated)
Reproductive - Specific Developmental Abnormalities - urogenital system.
Reproductive - Effects on Newborn - weaning or lactation index (e.g., # alive at weaning per # alive at day 4).

Reproductive - Effects on embryo or fetus - maternal/fetal exchange.
Reproductive - Specific Developmental Abnormalities - Central Nervous System.
Product name: Caffeine

Reproductive - Specific Developmental Abnormalities - eye/ear.
Reproductive - Effects on Newborn - viability index (e.g., # alive at day 4 per # born live).
Reproductive - Specific Developmental Abnormalities - hepato-biliary system.
Reproductive - Effects on Newborn - growth statistics (e.g., % reduced weight gain).
Reproductive - Specific Developmental Abnormalities - other developmental abnormalities.
Reproductive - Fertility - post-implantation mortality (e.g., dead/or resorbed implants per total number of implants).
Reproductive - Fertility - litter size (e.g., # fetuses per litter; measured before birth).
Reproductive - Effects on Embryo or Fetus - eye.
Reproductive - Specific Developmental Abnormalities - eye.
Reproductive - Specific Developmental Abnormalities - skin and skin appendages.
Reproductive - Effects on Newborn - sex ratio.
Reproductive - Effects on Newborn - live birth index (measured after birth).
Reproductive - Effects on Newborn - other neonatal measures or effects.
Skin and Appendages - sweating.
Skin and Appendages - hair.
Skin and Appendages - tumors.
Tumorigenic - active as anti-cancer agent.
Tumorigenic - carcinogenic by RTECS criteria.
Tumorigenic - increased incidence of tumors in susceptible strains.
Tumorigenic - facilitates action of known carcinogen.
Tumorigenic - neoplastic by RTECS criteria.
Vascular - BP elevation not characterized in autonomic section.
Vascular - regional or general arteriolar or venous dilation.

Additional toxicological information:
To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.
IARC-3: Not classifiable as to carcinogenicity to humans.

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

13 Disposal considerations
Product:
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.
Recommended cleansing agent: Water, if necessary with cleansing agents.

14 Transport information
DOT regulations:

Hazard class: 6.1
Identification number: UN1544
Packing group: III
Proper shipping name (technical name): ALKALOIDS, SOLID, N.O.S. (Caffeine)
Label 6.1

Land transport ADR/RID (cross-border)

ADR/RID class: 6.1 (T2) Toxic substances
Danger code (Kemler): 60
UN-Number: 1544
Packaging group: III
**Product name: Caffeine**

**Description of goods:** 1544 ALKALOIDS, SOLID, N.O.S. (Caffeine)

**Maritime transport IMDG:**

<table>
<thead>
<tr>
<th>IMDG Class</th>
<th>UN Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1</td>
<td>1544</td>
</tr>
</tbody>
</table>

**Label:** 6.1

**Packaging group:** III

**Proper shipping name:** ALKALOIDS, SOLID, N.O.S. (Caffeine)

**Air transport ICAO-TI and IATA-DGR:**

<table>
<thead>
<tr>
<th>ICAO/IATA Class</th>
<th>UN/ID Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1</td>
<td>1544</td>
</tr>
</tbody>
</table>

**Label:** 6.1

**Packaging group:** III

**Proper shipping name:** ALKALOIDS, SOLID, N.O.S. (Caffeine)

**UN "Model Regulation":** UN1544, ALKALOIDS, SOLID, N.O.S., 6.1, III

**15 Regulations**

**Product related hazard informations:**

**Hazard symbols:**

Xn Harmful

**Risk phrases:**

22 Harmful if swallowed.

**National regulations**

All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.

All components of this product are listed on the Canadian Domestic Substances List (DSL).

**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.

**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 MSDS:** Health, Safety and Environmental Department.

**Contact:** Zachariah Holt

**Abbreviations and acronyms:**

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

HMIS: Hazardous Materials Identification System (USA)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent