

## 1 Identification

- **Product identifier**
- **Trade name:** 3-Isobutyl-1-methylxanthine BioChemica
- **Article number:** A0695
- **CAS Number:**  
28822-58-4
- **EC number:**  
249-259-3
- **Application of the substance / the mixture**  
Biochemistry  
Laboratory chemical
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**  
AppliChem GmbH  
Ottoweg 4  
D-64291 Darmstadt
- **Information department:** Dept. Compliance
- **Emergency telephone number:** +49(0)6151 93570 (Inside normal business hours)

Tel.: +49 (0)6151 93570  
Fax.: +49 (0)6151 935711  
msds@applichem.com

## 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**



GHS07

- **Signal word** Warning
- **Hazard-determining components of labeling:**  
3-Isobutyl-1-methylxanthine BioChemica
- **Hazard statements**  
H302 Harmful if swallowed.
- **Precautionary statements**  
P313 Get medical advice/attention.  
P301+P330+P331 If swallowed: Rinse mouth. Do NOT induce vomiting.
- **Classification system:**
- **NFPA ratings (scale 0 - 4)**



Health = 2  
Fire = 0  
Reactivity = 0

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· **HMIS-ratings (scale 0 - 4)**

HEALTH	2	Health = 2
FIRE	0	Fire = 0
REACTIVITY	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**  
28822-58-4 3-Isobutyl-1-methylxanthine BioChemica
- **Identification number(s)**
- **EC number:** 249-259-3

### 4 First-aid measures

- **Description of first aid measures**
- **After inhalation:** Supply fresh air; consult doctor in case of complaints.
- **After skin contact:**  
Wash with water and acidic soap.  
Seek medical treatment.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **After swallowing:**  
Rinse out mouth.  
Seek medical treatment.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed** 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:**  
CO<sub>2</sub>, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **Special hazards arising from the substance or mixture**  
Formation of toxic gases is possible during heating or in case of fire.  
In case of fire, the following can be released:  
Nitrogen oxides (NO<sub>x</sub>)  
CO, CO<sub>2</sub>
- **Advice for firefighters**
- **Protective equipment:** Wear self-contained respiratory protective device.
- **Additional information**  
Dispose of fire debris and contaminated fire fighting water in accordance with official regulations.

### 6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**  
Avoid formation of dust.  
Do not inhale dust.  
Avoid substance contact.

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- *Ensure adequate ventilation*
- **Environmental precautions:** *Do not allow to enter sewers/ surface or ground water.*
- **Methods and material for containment and cleaning up:**
  - Pick up mechanically.*
  - Avoid generation of dusts.*
  - Dispose contaminated material as waste according to item 13.*
  - Clean up affected area.*
- **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** *Any deposit of dust which cannot be avoided must be regularly removed.*
- **Information about protection against explosions and fires:** *No special measures required.*
- **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:** *Not required.*
- **Further information about storage conditions:**
  - Store under lock and key and with access restricted to technical experts or their assistants only.*
  - Keep container sealed.*
- **Recommended storage temperature:** *2-8 °C*
- **Storage class:** *13*
- **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:** *Not required.*
- **Additional information:** *The lists that were valid during the creation were used as basis.*
- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**
  - Keep away from foodstuffs, beverages and feed.*
  - Wash hands before breaks and at the end of work.*
  - Vacuum clean contaminated clothing. Do not blow or brush off contamination.*
  - Change contaminated clothing.*
- **Breathing equipment:**
  - In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.*
  - Filter P1*
- **Protection of hands:**
  - The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.*
  - 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.*

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- **For the permanent contact gloves made of the following materials are suitable:**  
Nitrile rubber, NBR  
Recommended thickness of the material:  $\geq 0.11$  mm  
Value for the permeation: Level  $\geq 480$  min
- **As protection from splashes gloves made of the following materials are suitable:**  
Nitrile rubber, NBR  
Recommended thickness of the material:  $\geq 0.11$  mm  
Value for the permeation: Level  $\geq 480$  min
- **Eye protection:** Safety glasses
- **Body protection:**  
Protective clothing should be selected specifically for the working place, depending on concentration and quantity of the hazardous substances handled.

## 9 Physical and chemical properties

- **Information on basic physical and chemical properties**
- **General Information**
- **Appearance:**
  - **Form:** Solid
  - **Color:** Light yellow
  - **Odor:** No data available
  - **Odor threshold:** Not determined.
- **pH-value:** Not applicable.
- **Change in condition**
  - **Melting point/Melting range:** 200 - 203 °C (392 - 397 °F)
  - **Boiling point/Boiling range:** Undetermined.
- **Flash point:** Not applicable.
- **Flammability (solid, gaseous):** Product is not flammable.
- **Ignition temperature:**
  - **Decomposition temperature:** Not determined.
  - **Auto igniting:** Not determined.
- **Danger of explosion:** Product does not present an explosion hazard.
- **Explosion limits:**
  - **Lower:** Not determined.
  - **Upper:** Not determined.
- **Vapor pressure:** Not applicable.
- **Density:** Not determined.
- **Relative density** Not determined.
- **Vapor density** Not applicable.
- **Evaporation rate** Not applicable.
- **Solubility in / Miscibility with**
  - **Water:** Insoluble.
- **Partition coefficient (n-octanol/water):** Not determined.
- **Viscosity:**
  - **Dynamic:** Not applicable.
  - **Kinematic:** Not applicable.
- **Solvent content:**
  - **Organic solvents:** 0.0 %
  - **VOC content:** 0.0 g/l / 0.00 lb/gl

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· **Other information** 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 oxidants
- **Hazardous decomposition products:** In the event of fire: See chapter 5

### 11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**
- **Primary irritant effect:**
  - **on the skin:** No data available
  - **on the eye:** No data available.
- **Sensitization:**
  - Sensitizing effect through inhalation is possible with prolonged exposure.
  - Sensitizing effect by skin contact is possible with prolonged exposure.
- **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

- **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:**
  - Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.
  - Water hazard class 1 (Self-assessment): slightly hazardous for water
  - Do not allow to enter waters, waste water, or soil.
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Other adverse effects** No further relevant information available.

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### 13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**  
Chemicals must be disposed of in compliance with the respective national regulations.  
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.  
Packagings that cannot be cleansed are to be disposed of in the same manner as the product.

### 14 Transport information

- |  |  |
|--|--|
| · <b>UN-Number</b>   | Void   |
| · <b>DOT, ADR, ADN, IMDG, IATA</b>   | Void   |
| · <b>UN proper shipping name</b>   | Void   |
| · <b>DOT, ADR, ADN, IMDG, IATA</b>   | Void   |
| · <b>Transport hazard class(es)</b>  | Void   |
| · <b>DOT, ADR, ADN, IMDG, IATA</b>   | Void   |
| · <b>Class</b>   | Void   |
| · <b>Packing group</b>   | Void   |
| · <b>DOT, ADR, IMDG, IATA</b>  | Void   |
| · <b>Environmental hazards:</b>  |  |
| · <b>Marine pollutant:</b>   | No   |
| · <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>Transport/Additional information:</b>                                       | Not dangerous according to the above specifications. |
| · <b>UN "Model Regulation":</b>  | Void   |

### 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.

· **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.

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· **Chemicals known to cause developmental toxicity:**

Substance is not listed.

· **Carcinogenicity 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-determining components of labeling:**

3-Isobutyl-1-methylxanthine BioChemica

· **Hazard statements**

H302 Harmful if swallowed.

· **Precautionary statements**

P313 Get medical advice/attention.

P301+P330+P331 If swallowed: Rinse mouth. Do NOT induce vomiting.

· **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:** Dept. Compliance

· **Contact:** Mr. Th. Stöckle

· **Date of preparation / last revision** 10/06/2016 / 1

· **Abbreviations and acronyms:**

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

ICAO: International Civil Aviation Organisation

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

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)

VOC: Volatile Organic Compounds (USA, EU)

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