SAFETY DATA SHEET
3-Isobutyl-1-methylxanthine

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier
Product name 3-Isobutyl-1-methylxanthine
Product number FI24659
Synonyms; trade names 3,9-Dihydro-1-methyl-3-(2-methylpropyl)-1H-purine-2,6-dione, IBMX, 1-Methyl-3-isobutylxanthine
CAS number 28822-58-4

1.2. Relevant identified uses of the substance or mixture and uses advised against
Identified uses Laboratory reagent. Manufacture of substances. Research and development.

1.3. Details of the supplier of the safety data sheet
Supplier Carbosynth Ltd
8&9 Old Station Business Park
Compton
Berkshire
RG20 6NE
UK
+44 1635 578444
+44 1635 579444
info@carbosynth.com

1.4. Emergency telephone number
Emergency telephone +44 7887 998634

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture
Classification (EC 1272/2008)
Physical hazards Not Classified
Health hazards Acute Tox. 4 - H302
Environmental hazards Not Classified

2.2. Label elements
Pictogram

Signal word Warning
Hazard statements H302 Harmful if swallowed.
3-Isobutyl-1-methylxanthine

Precautionary statements
P264 Wash contaminated skin thoroughly after handling.
P301+P312 IF SWALLOWED: Call a POISON CENTRE/doctor if you feel unwell.
P330 Rinse mouth.
P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards
No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances
Product name 3-Isobutyl-1-methylxanthine
CAS number 28822-58-4
Chemical formula C₁₀H₁₄N₄O₂

SECTION 4: First aid measures

4.1. Description of first aid measures
General information Get medical advice/attention if you feel unwell.
Inhalation Remove person to fresh air and keep comfortable for breathing. If breathing stops, provide artificial respiration. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention if symptoms are severe or persist.
Ingestion Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.
Skin contact Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.
Eye contact Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

4.2. Most important symptoms and effects, both acute and delayed
General information See Section 11 for additional information on health hazards.

4.3. Indication of any immediate medical attention and special treatment needed
Notes for the doctor Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media
Suitable extinguishing media Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

5.2. Special hazards arising from the substance or mixture
Specific hazards None known.
Hazardous combustion products Thermal decomposition or combustion products may include the following substances: Oxides of carbon. Oxides of nitrogen.

5.3. Advice for firefighters
3-Isobutyl-1-methylxanthine

Special protective equipment for firefighters
Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures
Personal precautions
Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material.

6.2. Environmental precautions
Environmental precautions
Avoid discharge into drains or watercourses or onto the ground.

6.3. Methods and material for containment and cleaning up
Methods for cleaning up
Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

6.4. Reference to other sections
Reference to other sections
For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling
Usage precautions
Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid generation and spreading of dust. Avoid contact with skin and eyes. Avoid inhalation of dust and vapours.

7.2. Conditions for safe storage, including any incompatibilities
Storage precautions
Keep container tightly closed. Store at temperatures not exceeding -20°C.

7.3. Specific end use(s)
Specific end use(s)
The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure Controls/personal protection

8.1. Control parameters
Occupational exposure limits
No exposure limits known for ingredient(s).

8.2. Exposure controls
Appropriate engineering controls
Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection
Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.

Hand protection
Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.

Other skin and body protection
Wear appropriate clothing to prevent repeated or prolonged skin contact.
3-Isobutyl-1-methylxanthine

**Respiratory protection**
Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is ‘CE’-marked. Particulate filters should comply with European Standard EN143. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

**Environmental exposure controls**
Keep container tightly sealed when not in use.

### SECTION 9: Physical and Chemical Properties

#### 9.1. Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
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<td>Appearance</td>
<td>Solid</td>
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<td>Odour</td>
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<tr>
<td>Odour threshold</td>
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<tr>
<td>pH</td>
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<td>Melting point</td>
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<td>Initial boiling point and range</td>
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<td>Flash point</td>
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<td>Evaporation rate</td>
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<td>Flammability (solid, gas)</td>
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<td>Upper/lower flammability or explosive limits</td>
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<td>Vapour pressure</td>
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<td>Solubility(ies)</td>
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<td>Partition coefficient</td>
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<td>Auto-ignition temperature</td>
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<td>Decomposition Temperature</td>
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<td>Viscosity</td>
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<td>Explosive properties</td>
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<td>Oxidising properties</td>
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#### 9.2. Other information

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<td>Molecular weight</td>
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### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

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<th>Property</th>
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<tbody>
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<td>Reactivity</td>
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#### 10.2. Chemical stability

<table>
<thead>
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<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Stability</td>
<td>Stable under the prescribed storage conditions.</td>
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</table>
### 3-Isobutyl-1-methylxanthine

#### 10.3. Possibility of hazardous reactions

**Possibility of hazardous reactions**  
No data available.

#### 10.4. Conditions to avoid

**Conditions to avoid**  
No data available.

#### 10.5. Incompatible materials

**Materials to avoid**  
Strong oxidising agents.

#### 10.6. Hazardous decomposition products

**Hazardous decomposition products**  

### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

**Acute toxicity - oral**  
*Notes (oral LD₅₀)*  
Acute Tox. 4 - H302 Harmful if swallowed.

*ATE oral (mg/kg)*  
500.0

**Acute toxicity - dermal**  
*Notes (dermal LD₅₀)*  
Based on available data the classification criteria are not met.

**Acute toxicity - inhalation**  
*Notes (inhalation LC₅₀)*  
Based on available data the classification criteria are not met.

**Skin corrosion/irritation**  
*Animal data*  
Based on available data the classification criteria are not met.

**Serious eye damage/irritation**  
Based on available data the classification criteria are not met.

**Respiratory sensitisation**  
Based on available data the classification criteria are not met.

**Skin sensitisation**  
Based on available data the classification criteria are not met.

**Germ cell mutagenicity**  
Based on available data the classification criteria are not met.

**Carcinogenicity**  
Based on available data the classification criteria are not met.

**IARC carcinogenicity**  
None of the ingredients are listed or exempt.

**Reproductive toxicity**  
Based on available data the classification criteria are not met.

**Reproductive toxicity - fertility**  
Based on available data the classification criteria are not met.

**Reproductive toxicity - development**  
Based on available data the classification criteria are not met.

**Specific target organ toxicity - single exposure**  
STOT - single exposure  
Not classified as a specific target organ toxicant after a single exposure.

**Specific target organ toxicity - repeated exposure**
3-Isobutyl-1-methylxanthine

STOT - repeated exposure  Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard  Not relevant. Solid.

General information  Dust may irritate the eyes and the respiratory system. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation  Dust may irritate the respiratory system. Frequent inhalation of dust over a long period of time increases the risk of developing lung diseases.

Ingestion  May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.

Skin contact  Prolonged contact may cause dryness of the skin.

Eye contact  Dust may cause slight irritation.

Route of exposure  Ingestion Inhalation Skin and/or eye contact

Target organs  No specific target organs known.

RTECS #  ZD8500000

SECTION 12: Ecological Information

Ecotoxicity  Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity

Toxicity  Based on available data the classification criteria are not met.

12.2. Persistence and degradability

Persistence and degradability  The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential  No data available on bioaccumulation.

Partition coefficient  No data available.

12.4. Mobility in soil

Mobility  No data available.

12.5. Results of PBT and vPvB assessment

Results of PBT and vPvB assessment  No data available.

12.6. Other adverse effects

Other adverse effects  None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information  Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

SECTION 14: Transport information
3-Isobutyl-1-methylxanthine

General
The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).

14.1. UN number
Not applicable.

14.2. UN proper shipping name
Not applicable.

14.3. Transport hazard class(es)
No transport warning sign required.

14.4. Packing group
Not applicable.

14.5. Environmental hazards
Environmentally hazardous substance/marine pollutant
No.

14.6. Special precautions for user
Not applicable.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not applicable.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations
Health and Safety at Work etc. Act 1974 (as amended).
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) [*CDG 2009*].
EH40/2005 Workplace exposure limits.

EU legislation

15.2. Chemical safety assessment
No chemical safety assessment has been carried out.

SECTION 16: Other information
3-Isobutyl-1-methylxanthine

Abbreviations and acronyms used in the safety data sheet
ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
IATA: International Air Transport Association.
IMDG: International Maritime Dangerous Goods.
CAS: Chemical Abstracts Service.
ATE: Acute Toxicity Estimate.
LC₅₀: Lethal Concentration to 50 % of a test population.
LD₅₀: Lethal Dose to 50% of a test population (Median Lethal Dose).
EC₅₀: 50% of maximal Effective Concentration.
PBT: Persistent, Bioaccumulative and Toxic substance.
vPvB: Very Persistent and Very Bioaccumulative.

Training advice
Only trained personnel should use this material.

Revision date
29/01/2019

Revision
1

SDS number
144926

Hazard statements in full
H302 Harmful if swallowed.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.