

# SAFETY DATA SHEET

## 1. PRODUCT

### 1.1 Product identifiers

Name: 3-Isobutyl-1-methylxanthine

CAS-No.: 28822-58-4

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

## 2. HAZARDS IDENTIFICATION


### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 4), H302

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal word	Warning
Hazard statement(s)	H302 Harmful if swallowed.
Precautionary statement(s)	P264 Wash skin thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P301 + P312 IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell. P330 Rinse mouth. P501 Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

No data available

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms: IBMX  
3-Isobutyl-1-methyl-2,6(1H,3H)-purinedione  
3,7-Dihydro-1-methyl-3-(2-methylpropyl)-1H-purine-2,6-dione  
1-Methyl-3-isobutylxanthine

Formula:  $C_{10}H_{14}N_4O_2$

CAS-No.: 28822-58-4

EC-No.: 249-259-3

#### Hazardous components

Component	Classification	Concentration
<b>3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione</b>		
	Acute Tox. 4; H302	-

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

<b>General advice</b>
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
<b>If inhaled</b>
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
<b>In case of skin contact</b>
Wash off with soap and plenty of water. Consult a physician.
<b>In case of eye contact</b>
Flush eyes with water as a precaution.
<b>If swallowed</b>
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### 4.2 Indication of any immediate medical attention and special treatment needed

no data available

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides, nitrogen oxides (NO<sub>x</sub>)

### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

### 5.4 Further information

no data available

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

## 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

## 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature: -20 °C

Keep in a dry place.

## 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

Eye/face protection	Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Skin protection	Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. Full contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M) Splash contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M) data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374 If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.
Body Protection	Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
Respiratory protection	For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).
Control of environmental exposure	Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

Appearance	Form: powder Colour: light yellow
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Odour	no data available
Odour Threshold	no data available
pH	no data available
Melting point/freezing point	Melting point/range: 200 - 201 °C (392 - 394 °F)
Initial boiling point and boiling range	no data available
Flash point	no data available
Evaporation rate	no data available
Flammability (solid, gas)	no data available
Upper/lower flammability or explosive limits	no data available
Vapour pressure	no data available
Vapour density	no data available
Relative density	no data available
Water solubility	no data available
Partition coefficient: n-octanol/water	log Pow: 1.582
Auto-ignition temperature	no data available
Decomposition temperature	no data available
Viscosity	no data available
Explosive properties	no data available
Oxidizing properties	no data available

## 9.2 Other safety information

no data available

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

no data available

### 10.4 Conditions to avoid

no data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

<b>Acute toxicity</b>
Inhalation: no data available Dermal: no data available LD50 Intraperitoneal - mouse - 44 mg/kg
<b>Skin corrosion/irritation</b>
no data available
<b>Serious eye damage/eye irritation</b>
no data available

<b>Respiratory or skin sensitisation</b>
no data available
<b>Germ cell mutagenicity</b>
no data available
<b>Carcinogenicity</b>
IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH. NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP. OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
<b>Reproductive toxicity</b>
no data available no data available
<b>Specific target organ toxicity -single exposure</b>
no data available
<b>Specific target organ toxicity -repeated exposure</b>
no data available
<b>Aspiration hazard</b>
no data available
<b>Additional Information</b>
RTECS: ZD8500000 To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Liver - Irregularities - Based on Human Evidence Liver - Irregularities - Based on Human Evidence

## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

no data available

### 12.2 Persistence and degradability

no data available

### 12.3 Bioaccumulative potential

no data available

### 12.4 Mobility in soil

no data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Other adverse effects

no data available

## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

<b>Product</b>
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.
<b>Contaminated packaging</b>
Dispose of as unused product.

## 14. TRANSPORT INFORMATION

### DOT (US)

Not dangerous goods

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

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## 15. REGULATORY INFORMATION

### SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know Components

Component	CAS-No.	Revision Date
3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione	28822-58-4	

### New Jersey Right To Know Components

Component	CAS-No.	Revision Date
3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione	28822-58-4	

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity

H302 Harmful if swallowed.

### HMIS Rating

Health hazard: 2

Chronic Health Hazard: \*

Flammability: 0

Physical Hazard 0

### NFPA Rating

Health hazard: 2

Fire Hazard: 0

Reactivity Hazard: 0

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