

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : 3-Isobutyl-1-methylxanthine
Product Number : I5879
Brand : Sigma
Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
Telephone : +1 800-325-5832
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Emergency Phone # : (314) 776-6555

ORNL INTERNAL USE ONLYRECID A0569DATE 3/31/09**2. COMPOSITION/INFORMATION ON INGREDIENTS**

Synonyms : 1-Methyl-3-isobutylxanthine
3,7-Dihydro-1-methyl-3-(2-methylpropyl)-1H-purine-2,6-dione
3-Isobutyl-1-methyl-2,6(1H,3H)-purinedione
IBMX
Formula : C₁₀H₁₄N₄O₂
Molecular Weight : 222.25 g/mol

| CAS-No. | EC-No. | Index-No. | Concentration |
|--|-----------|-----------|---------------|
| 3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione | | | |
| 28822-58-4 | 249-259-3 | - | - |

3. HAZARDS IDENTIFICATION**Emergency Overview****OSHA Hazards**

Delayed target organ effects

Toxic by ingestion

Target Organs

Nerves., Heart, Kidney

HMS Classification

Health Hazard: 2

Chronic Health Hazard: *

Flammability: 0

Physical hazards: 0

NFPA Rating

Health Hazard: 2

Fire : 0

Reactivity Hazard: 0

Potential Health Effects

| | |
|-------------------|---|
| Inhalation | May be harmful if inhaled. May cause respiratory tract irritation. |
| Skin | May be harmful if absorbed through skin. May cause skin irritation. |
| Eyes | May cause eye irritation. |
| Ingestion | Toxic if swallowed. |

4. FIRST AID MEASURES

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIRE-FIGHTING MEASURES

Flammable properties

Flash point no data available

Ignition temperature no data available

Suitable extinguishing media

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

Special protective equipment for fire-fighters

Wear self contained breathing apparatus for fire fighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

Use personal protective equipment. Avoid dust formation. Avoid breathing dust. Ensure adequate ventilation.

Environmental precautions

Do not let product enter drains.

Methods for cleaning up

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

7. HANDLING AND STORAGE

Handling

Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Storage

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

Recommended storage temperature: -20 °C

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection

Handle with gloves.

Eye protection

Safety glasses

Skin and body protection

Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Hygiene measures

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

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

| | |
|--------|--------------|
| Form | powder |
| Colour | light yellow |

Safety data

| | |
|---|-------------------|
| pH | no data available |
| Melting point | 201 °C (394 °F) |
| Boiling point | no data available |
| Flash point | no data available |
| Ignition temperature | no data available |
| Lower explosion limit | no data available |
| Upper explosion limit | no data available |
| Water solubility | no data available |
| Partition coefficient: n-octanol/water | log Pow: 1.582 |

10. STABILITY AND REACTIVITY

Storage stability

Stable under recommended storage conditions.

Materials to avoid

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO_x)

11. TOXICOLOGICAL INFORMATION

Acute toxicity

LD50 Intraperitoneal - mouse - 44 mg/kg

Irritation and corrosion

no data available

Sensitisation

no data available

Chronic exposure

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.

Signs and Symptoms of Exposure

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Potential Health Effects

| | |
|----------------------|---|
| Inhalation | May be harmful if inhaled. May cause respiratory tract irritation. |
| Skin | May be harmful if absorbed through skin. May cause skin irritation. |
| Eyes | May cause eye irritation. |
| Ingestion | Toxic if swallowed. |
| Target Organs | Nerves., Heart, Kidney, |

12. ECOLOGICAL INFORMATION**Elimination information (persistence and degradability)**

no data available

Ecotoxicity effects

no data available

Further information on ecology

no data available

13. DISPOSAL CONSIDERATIONS**Product**

Observe all federal, state, and local environmental regulations. 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.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION**DOT (US)**

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

15. REGULATORY INFORMATION

OSHA Hazards

Delayed target organ effects, Toxic by ingestion

TSCA Status

Not On TSCA Inventory

3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione

CAS-No.
28822-58-4

DSL Status

This product contains the following components that are not on the Canadian DSL nor NDSL lists.

3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione

CAS-No.
28822-58-4

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 Listed

Pennsylvania Right To Know Components

3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione

CAS-No. Revision Date
28822-58-4

New Jersey Right To Know Components

3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione

CAS-No. Revision Date
28822-58-4

California Prop. 65 Components

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

16. OTHER INFORMATION

Further information

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