


SAFETY DATA SHEET

Version 3.11
Revision Date 06/16/2014
Print Date 06/17/2015

1. PRODUCT AND COMPANY IDENTIFICATION

- 1.1 Product identifiers**
Product name : 3-Isobutyl-1-methylxanthine
- Product Number : I5879
Brand : Sigma
- 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
- 1.3 Details of the supplier of the safety data sheet**
Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA
- Telephone : +1 800-325-5832
Fax : +1 800-325-5052
- 1.4 Emergency telephone number**
Emergency Phone # : (314) 776-6555

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 - none**

3. COMPOSITION/INFORMATION ON INGREDIENTS

- 3.1 Substances**
Synonyms : IBMX
- Sigma - I5879
- Delivery 0850863018-000020 Purchase Order 8015MU490

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 : C₁₀H₁₄N₄O₂
Molecular Weight : 222.24 g/mol
CAS-No. : 28822-58-4
EC-No. : 249-259-3

Hazardous components

Component	Classification	Concentration
3,7-Dihydro-3-isobutyl-1-methyl-1h-purine-2,6-dione	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**
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**
Flush eyes with water as a precaution.
- If swallowed**
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
- 4.3 Indication of any immediate medical attention and special treatment needed**
no data available

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 (NOx)
- 5.3 Advice for firefighters**
Wear self contained breathing apparatus for fire fighting if necessary.
- 5.4 Further information**
no data available

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.

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Safety

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.

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

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: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: powder Colour: light yellow
b) Odour	no data available
c) Odour Threshold	no data available
d) pH	no data available
e) Melting point/freezing point	Melting point/range: 200 - 201 °C (392 - 394 °F)
f) Initial boiling point and boiling range	no data available
g) Flash point	no data available
h) Evaporation rate	no data available
i) Flammability (solid, gas)	no data available
j) Upper/lower flammability or explosive limits	no data available
k) Vapour pressure	no data available
l) Vapour density	no data available
m) Relative density	no data available
n) Water solubility	no data available
o) Partition coefficient: n-octanol/water	log Pow: 1.582
p) Auto-ignition temperature	no data available
q) Decomposition temperature	no data available
r) Viscosity	no data available
s) Explosive properties	no data available
t) 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

Acute toxicity

Inhalation: no data available

Dermal: no data available

LD50 Intraperitoneal - mouse - 44 mg/kg

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

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.

Reproductive toxicity

no data available

no data available

Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

no data available

Additional information

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

Product

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.

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

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

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

CAS-No.
28822-58-4

Revision Date

New Jersey Right To Know Components

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

CAS-No.
28822-58-4

Revision Date

California Prop. 65 Components

00000277

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Delivery 0850863018-000020 Purchase Order 8015MU490

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

16. OTHER INFORMATION

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

Acute Tox.	Acute toxicity
H302	Harmful if swallowed.

HMS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

Further Information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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