

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

Product name : 1,7-Dimethylxanthine

2. HAZARDS IDENTIFICATION

Classification of the substance or mixture

According to Regulation (EC) No1272/2008
Acute toxicity, Oral (Category 4)

According to European Directive 67/548/EEC as amended.
Harmful if swallowed.

Label elements

Pictogram	
Signal word	Warning
Hazard statement(s) H302	Harmful if swallowed.
Precautionary statement(s)	none
Hazard symbol(s) Xn	Harmful
R-phrases(s) R22	Harmful if swallowed.
S-phrases(s)	none

Other hazards - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 1,7-Dimethyl-1H-purine-2,6-dione
2,6-Dihydroxy-1,7-dimethylpurine
Paraxanthine
3,7-dihydro-1,7-dimethyl-1H-purine-2,6-dione

Formula : C7H8N4O2
Molecular Weight : 180,16 g/mol

CAS-No.	EC-No.	Classification	Concentration
3,7-dihydro-1,7-dimethyl-1H-purine-2,6-dione 611-59-6	210-271-9	- Acute Tox. 4; H302 Xn, R22	-

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

4. FIRST AID MEASURES

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

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

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 and materials for containment and cleaning up

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

7. HANDLING AND STORAGE

Precautions for safe handling

Avoid formation of dust and aerosols.
Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Conditions for safe storage

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

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

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Handle with gloves.

Eye protection

Safety glasses with side-shields conforming to EN166

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 crystalline

Safety data

pH no data available
Melting point 294 - 296 °C
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 1 g/l
Partition coefficient:
n-octanol/water log Pow: -0,687
Solubility 0,6 g/l Ethanol

10. STABILITY AND REACTIVITY

Chemical stability

Stable under recommended storage conditions.

Conditions to avoid

no data available

Materials to avoid

Strong oxidizing agents

Hazardous decomposition products

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

11. TOXICOLOGICAL INFORMATION

Acute toxicity

no data available

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitization

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.

Reproductive toxicity

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

Potential health effects

Inhalation May be harmful if inhaled. May cause respiratory tract irritation.

Ingestion Harmful if swallowed.

Skin May be harmful if absorbed through skin. May cause skin irritation.

Eyes May cause eye irritation.

Signs and Symptoms of Exposure

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

Additional Information

RTECS: RV9380000

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

PBT and vPvB assessment

no data available

Other adverse effects

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

ADR/RID

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

16. OTHER INFORMATION

Text of H-code(s) and R-phrases mentioned in Section 3

Acute Tox. Acute toxicity
H302 Harmful if swallowed.
Xn Harmful
R22 Harmful if swallowed.

Further information

For R&D use only. Not for drug, household or other uses.

WARRANTY:

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Lookchem shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.