

SAFETY DATA SHEET

Creation Date 09-Jul-2012

Revision Date 14-Feb-2020

Revision Number 2

1. Identification

Product Name 3-Methylxanthine

Cat No. : L14986

CAS-No 1076-22-8
Synonyms 2,6-Dihydroxy-3-methylpurine

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.
Details of the supplier of the safety data sheet

Company

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Emergency Telephone Number

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660.
After normal business hours, call Carechem 24 at (866) 928-0789.

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity Category 4

Label Elements

Signal Word

Warning

Hazard Statements

Harmful if swallowed

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
3,7-Dihydro-3-methyl-1H-purine-2,6-dione	1076-22-8	>95

4. First-aid measures

General Advice	If symptoms persist, call a physician.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	No information available
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	No information available

Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

Environmental Precautions Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

7. Handling and storage

Handling Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid dust formation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.

Storage Keep containers tightly closed in a dry, cool and well-ventilated place.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection No protective equipment is needed under normal use conditions.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State Solid
Appearance No information available

Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	> 300 °C / > 572 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	Not applicable
Molecular Formula	C6 H6 N4 O2
Molecular Weight	166.14

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Avoid dust formation. Incompatible products. Excess heat.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Nitrogen oxides (NOx)
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Toxicologically Synergistic Products	No information available
--------------------------------------	--------------------------

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
3,7-Dihydro-3-methyl-1-H-purine-2,6-dione	1076-22-8	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects	No information available
-------------------	--------------------------

Reproductive Effects	No information available.
----------------------	---------------------------

Developmental Effects	No information available.
Teratogenicity	No information available.
STOT - single exposure	None known
STOT - repeated exposure	None known
Aspiration hazard	No information available
Symptoms / effects, both acute and delayed	No information available
Endocrine Disruptor Information	No information available
Other Adverse Effects	The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains. .

Persistence and Degradability	Persistence is unlikely
Bioaccumulation/ Accumulation	No information available.
Mobility	Is not likely mobile in the environment due its low water solubility.

Component	log Pow
3,7-Dihydro-3-methyl-1H-purine-2,6-dione	-0.698

13. Disposal considerations

Waste Disposal Methods	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
-------------------------------	---

14. Transport information

DOT	Not regulated
TDG	Not regulated
IATA	Not regulated
IMDG/IMO	Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS-No	TSCA	TSCA Inventory notification - Active/Inactive	TSCA - EPA Regulatory Flags
3,7-Dihydro-3-methyl-1H-purine-2,6-dione	1076-22-8	-	-	-

Legend:

TSCA - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export	Not applicable
---------------------------------------	----------------

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Australia (AICS), China (IECSC), Korea (ECL).

Component	CAS-No	DSL	NDSL	EINECS	PICCS	ENCS	AICS	IECSC	KECL
3,7-Dihydro-3-methyl-1H-purine-2,6-dione	1076-22-8	-	-	214-058-1	-	-	-	-	-

U.S. Federal Regulations

SARA 313	Not applicable
SARA 311/312 Hazard Categories	See section 2 for more information
CWA (Clean Water Act)	Not applicable
Clean Air Act	Not applicable
OSHA - Occupational Safety and Health Administration	Not applicable
CERCLA	Not applicable
California Proposition 65	This product does not contain any Proposition 65 chemicals.
U.S. State Right-to-Know Regulations	Not applicable
U.S. Department of Transportation	
Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N
U.S. Department of Homeland Security	This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade	No information available
-----------------------	--------------------------

16. Other information

Prepared By	Health, Safety and Environmental Department Email: tech@alfa.com www.alfa.com
Creation Date	09-Jul-2012
Revision Date	14-Feb-2020
Print Date	14-Feb-2020
Revision Summary	SDS authoring systems update, replaces ChemGes SDS No. 1076-22-8.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The 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, unless specified in the text

End of SDS