

ALFAAA12681

4,6-Dihydroxy-2-mercaptopyrimidine

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

产品说明: 4,6-二羟基-2-巯基嘧啶
Product Description: 4,6-Dihydroxy-2-mercaptopyrimidine

Cat No. : A12681
Synonyms 2-Thiobarbituric acid
CAS No 504-17-6
Molecular Formula C4 H4 N2 O2 S

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
Shore Road, Heysham
Lancashire, LA3 2XY,
United Kingdom
Office Tel: +44 (0) 1524 850506
Office Fax: +44 (0) 1524 850608

Emergency Telephone Number For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Powder Solid

Appearance
Off-white

Odor
Stench

Emergency Overview

Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation. Air sensitive. Stench.

Classification of the substance or mixture

Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

Label Elements



Signal Word

Warning

Hazard Statements

H315 - Causes skin irritation
 H319 - Causes serious eye irritation
 H335 - May cause respiratory irritation

Precautionary Statements**Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
 P264 - Wash face, hands and any exposed skin thoroughly after handling
 P271 - Use only outdoors or in a well-ventilated area
 P280 - Wear protective gloves/protective clothing/eye protection/face protection

Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
 P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
 P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
 P312 - Call a POISON CENTER or doctor if you feel unwell
 P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

None identified.

Health Hazards

Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

Other Hazards

Stench. Toxic to terrestrial vertebrates. This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
4,6(1H,5H)-Pyrimidinedione, dihydro-2-thioxo-	504-17-6	<=100

SECTION 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.

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

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.

SECTION 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.

Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

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

Storage

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

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and

SAFETY DATA SHEET

4,6-Dihydroxy-2-mercaptopyrimidine

inhalable dust

Exposure Controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

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

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Particulates filter conforming to EN 143

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Particle filtering: EN149:2001
When RPE is used a face piece Fit Test should be conducted

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

Environmental exposure controls No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance Off-white
Physical State Powder Solid

Odor Stench
Odor Threshold No data available
pH Not applicable
Melting Point/Range 240 - 255 °C / 464 - 491 °F
Softening Point No data available
Boiling Point/Range No information available
Flash Point No information available

Method - No information available

SAFETY DATA SHEET

4,6-Dihydroxy-2-mercaptopyrimidine

Evaporation Rate	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	Not applicable	Solid
Specific Gravity / Density	No data available	
Bulk Density	No data available	
Water Solubility	< 6 g/L (20 °C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	Not applicable	
Decomposition Temperature	No data available	
Viscosity	Not applicable	Solid
Explosive Properties	No information available	
Oxidizing Properties	No information available	
Molecular Formula	C4 H4 N2 O2 S	
Molecular Weight	144.15	

SECTION 10. STABILITY AND REACTIVITY

Stability	Air sensitive.
Hazardous Reactions	None under normal processing.
Hazardous Polymerization	No information available.
Conditions to Avoid	Incompatible products. Exposure to air.
Materials to avoid	Strong oxidizing agents.

Hazardous Decomposition Products Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
4,6(1H,5H)-Pyrimidinedione, dihydro-2-thioxo-	>5 g/kg (Rat)		

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;
Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available
 There are no known carcinogenic chemicals in this product

SAFETY DATA SHEET

4,6-Dihydroxy-2-mercaptopyrimidine

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3
Results / Target organs Respiratory system

(i) STOT-repeated exposure; No data available
Target Organs None known.

(j) aspiration hazard; Not applicable
Solid

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed No information available

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Do not empty into drains.

Persistence and Degradability
Persistence Soluble in water, Persistence is unlikely, based on information available.

Bioaccumulative Potential Bioaccumulation is unlikely

Mobility in soil The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility Highly mobile in soils

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport Not Regulated

Technical Shipping Name 4,6-Dihydroxy-2-mercaptopyrimidine

IMDG/IMO Not regulated

SAFETY DATA SHEET

4,6-Dihydroxy-2-mercaptopyrimidine

Technical Shipping Name 4,6-Dihydroxy-2-mercaptopyrimidine

IATA

UN-No UN3335
Proper Shipping Name AVIATION REGULATED SOLID, N.O.S.*
Technical Shipping Name 4,6-Dihydroxy-2-mercaptopyrimidine
Hazard Class 9
Packing Group III

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION

International Inventories

China, X = listed, Australia, U.S.A. (TSCA), Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Australia (AICS), Korea (KECL), China (IECSC), Japan (ENCS), Philippines (PICCS), Taiwan (TCSI), Japan (ISHL), New Zealand (NZIoC), Japan (ISHL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
4,6(1H,5H)-Pyrimidine dione, dihydro-2-thioxo-	-	-	X	X	207-985-8	X	X	X	-		X	KE-10756

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 12-Sep-2002
Revision Date 15-Sep-2025
Revision Summary SDS sections updated.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

SAFETY DATA SHEET

4,6-Dihydroxy-2-mercaptopyrimidine

DNEL - Derived No Effect Level
RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOEC - No Observed Effect Concentration
PBT - Persistent, Bioaccumulative, Toxic

PNEC - Predicted No Effect Concentration
LD50 - Lethal Dose 50%
EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water
vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road
OECD - Organisation for Economic Co-operation and Development
BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code
MARPOL - International Convention for the Prevention of Pollution from Ships
ATE - Acute Toxicity Estimate
VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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 Safety Data Sheet