

## 1: Identification of substance / mixture

## 1. Product Identifier

Substance

Product Name **5,6-Diamino-2-thioxo-2,3-dihydro-1H-pyrimidin-4-one**  
 Product Code 049441  
 CAS Number 1004-76-8  
 Other Names 4,5-Diamino-6-hydroxy-2-mercaptopyrimidine  
 IUPAC  
 MFCD Number MFCD00040963  
 EC/EINECS  
 REACH Number

## 2. Relevant identified uses of the substance or mixture and uses advised against

Research and Development

## 3. Details of the supplier of the safety data sheet

Fluorochem Ltd  
 Unit 14, Graphite Way  
 Hadfield  
 Derbyshire  
 SK13 1QH  
 UK



Telephone: +44(0)1457 892111  
 Fax number: +44(0)1457 892799  
 Email: MartinW@fluorochem.co.uk

## 4. Emergency telephone number

+44(0)1457 892134

## 2. Hazards Identification

## 1. Classification of the substance or mixture

H302	Acute Tox. 4	R22, R20/22, R20/21/22, R21/22, R68/20/22, R68/21/22, R68/20/21/22
H315	Skin Irrit. 2	R38, R36/38, R36/37/38, R37/38
H319	Eye Irrit. 2	R36, R36/37, R36/38, R36/37/38
H332	Acute Tox. 4	R20, R20/21, R20/22, R20/21/22, R68/20/21, R68/20/22, R68/20/21/22
H335	STOT SE 3a	R37, R36/37, R36/37/38, R37/38

\* The risk codes have been generated using Annex VII of directive 67/548/EEC. Risk code combinations are not included.

## 2. Label elements

Signal Word **Warning**

## Hazard Statements

H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.

## Precautionary Phrases

P264	Wash hands thoroughly after handling.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313	If skin irritation occurs: Get medical advice/attention.
P337 + P313	If eye irritation persists: Get medical advice/attention.

### 3. Other Hazards

Additional precautionary phrases are located throughout the safety data sheet

## 3. Composition / Information on Ingredients

### 1. Substances

5,6-Diamino-2-thioxo-2,3-dihydro-1H-pyrimidin-4-one

Assay:100% CAS Number :1004-76-8

### 2. Mixtures

Not Relevant

## 4. First Aid Measures

### 1. Description of first aid measures

<i>Skin Contact</i>	P302 + P352: IF ON SKIN: Wash with plenty of soap and water. P332 + P313: If skin irritation occurs: Get medical advice/attention.
<i>Eye Contact</i>	P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P337 + P313: If eye irritation persists: Get medical advice/attention.
<i>Ingestion</i>	Wash out mouth with water.
<i>Inhalation</i>	P304 + P340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

### 2. Most important symptoms and effects

No symptoms.

### 3. Indication of any immediate medical attention

P312: Call a POISON CENTER or doctor/physician if you feel unwell.  
No additional measures required

## 5. Firefighting measures

### 1. Extinguishing Media

<i>Suitable</i>	Carbon dioxide. Dry chemical powder. Water.
<i>Unsuitable</i>	Do not use water with a full water jet

### 2. Special Hazards arising from the substance or mixture

In combustion toxic fumes may form.

### 3. Advice for Fire Fighters

Wear protective clothing to prevent contact with skin and eyes.  
Wear self-contained breathing apparatus.

## 6. Accidental Release Measures

### 1. Personal Precautions

Refer to section 8 of SDS for personal protection details.

## 2.Environmental Precautions

Do not discharge into drains or rivers.

## 3.Methods & Materials

Mix with sand or vermiculite.  
Transfer to a suitable container.

## 7.Handling and Storage

### 1.Personnal Precautions

<i>Safe Handling</i>	Handle in fume hood. Wash hands immediately after contamination. P264: Wash hands thoroughly after handling.
<i>Protection against explosions and fires</i>	P362: Take off contaminated clothing and wash before reuse. normal measures for preventive fire protection

### 2.Conditions for safe storage, including any incompatibilities

<i>Managing Storage Risks</i>	Keep container tightly closed. Store in cool, well ventilated area.
<i>Storage Controls</i>	No special requirements
<i>Maintaining Integrity</i>	Keep in tightly closed container in cool area away from direct sunlight or heat sources.
<i>Other advice</i>	P403 + P233: Store in a well-ventilated place. Keep container tightly closed.

### 3.Specific End Uses

The end use(s) have not been fully determined. The substance is supplied for Research and Development purposes by professionals only.

## 8.Exposure Controls/Personal Protection

### 1. Control Parameters

Not Applicable

### 2.Exposure Controls

<i>General protective and hygiene measures</i>	P280: Wear protective gloves/protective clothing/eye protection/face protection. The standard precautionary measures should be adhered to when handling Wash hands during breaks and at the end of handling the material Immediately remove any contaminated clothing
<i>Engineering measures</i>	P271: Use only outdoors or in a well-ventilated area. Ensure there is sufficient ventilation of the area.
<i>Eye / Face Protection</i>	Safety Glasses.
<i>Hand protection</i>	Protective gloves.
<i>Respiratory protection</i>	

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P261: Avoid breathing dust/fume/gas/mist/vapours/spray.  
Respiratory protection not required.

*Skin protection* Protective clothing.

*Other personal protection advice* no data

## 9. Physical and Chemical Properties

### 1. Physical and Chemical Properties

Appearance	solid
Odour	Not Applicable
Odour threshold	Not Applicable
PH	Not Applicable
Melting point / Freezing point	> 300 °C - lit.
Initial boiling point and boiling range	Not Applicable
Flash point	Not Applicable
Evaporation rate	Not Applicable
Flammability(solid,gas)	Not Applicable
Upper/lower flammability or explosive limits	Not Applicable
Vapour pressure	Not Applicable
Vapour density	Not Applicable
Relative density	Not Applicable
Solubility(ies):	Not Applicable
Partition coefficient: n-octanol/water	Not Applicable
Auto-ignition temperature	Not Applicable
Decomposition temperature	Not Applicable
Viscosity	Not Applicable
Explosive properties	Not Applicable
Oxidising properties	Not Applicable

### 2. Other Information

No additional information available

## 10. Stability and Reactivity

### 1. Reactivity

no unusual reactivity

### 2. Stability

Stable under normal conditions.

### 3. Possibility of Hazardous Reactions

no hazardous reactions known

### 4. Conditions to Avoid

no specific conditions to avoid

### 5. Incompatible Materials

Strong oxidizing agents.

## 6. Hazardous Decomposition Products

In combustion emits toxic fumes.

## 11. Toxicology information

### 1. Information

<i>Acute Toxicity</i>	no data
<i>Skin corrosion/irritation</i>	irritant for skin and mucous membranes
<i>Serious eye Damage/irritation</i>	irritant effect
<i>Respiratory or skin sensitisation</i>	No sensitizing effect known
<i>Germ Cell mutagenicity</i>	not known
<i>Carcinogenicity</i>	not known
<i>Reproductive toxicity</i>	not known
<i>STOT-single exposure</i>	not known
<i>STOT-repeated exposure</i>	not known
<i>Aspiration hazard</i>	not known

### 2. Additional

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.  
No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH

## 12. Ecological Information

### 1. Toxicity

not known

### 2. Persistence and degradability

not known

### 3. Bio-Accumulative Potential

not known

### 4. Mobility and Soil

not known

### 5. Results of PBT & vPvB assessment

not known

### 6. Other adverse effects

not known

## 13. Disposal Considerations

## 1. Waste Treatment Methods

*Disposal Operations* Consult state, local or national regulations for proper disposal.  
Hand over to authorised disposal company as hazardous waste.

*Disposal of Packaging* Disposal must be made according to official regulations.

## 14. Transport Information

### Air (ICAO)

Not classified as hazardous for transport

### Road (ADR)

Not classified as hazardous for transport

### Sea (IMDG)

Not classified as hazardous for transport

## 15. Safety, health and environmental regulations

### 1. Safety, health and environmental regulations:

product is not subject to any additional regulations or provisions

### 2. Safety Assessment

No Chemical Safety Assessment

## 16. Other Information

### 1. Other Information:

ADR: Accord Europeen sur le transport des marchandises Dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by road)

RID: Reglement International concernant le transport des marchandises dangereuses par chemin de fer (Regulations concerning the International transport of Dangerous Goods by Rail)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

IATA-DGR: Dangerous Goods Regulations by the International Air Transport Association

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the ICAO

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

CAS: Chemical Abstracts Service

### 2. Associated risk phrases according to european directive 67/548/EEC

R20	Harmful by inhalation.
R20/21	Harmful by inhalation and in contact with skin.
R20/21/22	Harmful by inhalation, in contact with skin and if swallowed.
R20/22	Harmful by inhalation and if swallowed.

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R21/22	Harmful in contact with skin and if swallowed.
R22	Harmful if swallowed.
R36	Irritating to eyes.
R36/37	Irritating to eyes and respiratory system.
R36/37/38	Irritating to eyes, respiratory system and skin.
R36/38	Irritating to eyes and skin.
R37	Irritating to respiratory system.
R37/38	Irritating to respiratory system and skin.
R38	Irritating to skin.
R68/20/21	Harmful: possible risk of irreversible effects through inhalation and in contact with skin.
R68/20/21/22	Harmful: possible risk of irreversible effects through inhalation, in contact with skin and if swallowed.
R68/20/22	Harmful: possible risk of irreversible effects through inhalation and if swallowed.
R68/21/22	Harmful: possible risk of irreversible effects in contact with skin and if swallowed.



### 3. Disclaimer

The product listed is for research and development purposes only and not for human or animal use. As such, in most cases, the toxicological, ecological and physicochemical properties have not been fully determined and the product should be treated with respect and always handled under suitable conditions by appropriately qualified personnel. The responsible party shall use this datasheet only in conjunction with other sources of information gathered by them, and should make an independent judgement of suitability, to ensure proper use and protect the health and safety of employees. This information is furnished without warranty and any use of the product not in conformance with this material safety data sheet, or in combination with any other product or process, is the responsibility of the user.