

Chemical Safety Data Sheet MSDS / SDS

2-Mercapto-4-hydroxy-5,6-diaminopyrimidine

Revision Date:2026-05-31 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name : 2-Mercapto-4-hydroxy-5,6-diaminopyrimidine
CBnumber : CB3755761
CAS : 1004-76-8
EINECS Number : 213-727-5
Synonyms : 4,5-Diamino-6-hydroxy-2-mercaptopyrimidine,5,6-diamino-2,3-dihydro-2-thioxopyrimidin-4(1H)-one

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.
P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352 IF ON SKIN: wash with plenty of soap and water.
P321 Specific treatment (see ... on this label).
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.
P362 Take off contaminated clothing and wash before reuse.

Hazard statements

H335 May cause respiratory irritation

H315 Causes skin irritation

H319 Causes serious eye irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2-Mercapto-4-hydroxy-5,6-diaminopyrimidine
Synonyms	: 4,5-Diamino-6-hydroxy-2-mercaptopyrimidine,5,6-diamino-2,3-dihydro-2-thioxopyrimidin-4(1H)-one
CAS	: 1004-76-8
EC number	: 213-727-5
MF	: C4H6N4OS
MW	: 158.18

SECTION 4: First aid measures

4.1 Description of first aid measures

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Sulphur oxides

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

Storage class

Storage class (TRGS 510): 11: Combustible Solids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	Melting point/ range: > 300 °C - lit.
e) Initial boiling point and boiling range	No data available
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	No data available
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	1.66±0.1 g/cm ³ (Predicted)
Relative density	1.66±0.1 g/cm ³ (Predicted)
q) Relative vapour density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

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

SECTION 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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: -

IMDG: -

IATA: -

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA: -

14.4 Packaging group

ADR/RID: -

IMDG: -

IATA: -

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

No data available

Further information: Not classified as dangerous in the meaning of transport regulations.

14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No.

1907/2006.

International Chemical Weapons Convention : (CWC) Schedules of Toxic Chemicals and Precursors

Restrictions on the marketing and use of certain : dangerous substances and preparations

Regulation (EU) No 649/2012 of the European : Parliament and the Council concerning the export and import of dangerous chemicals

Candidate List of Substances of Very High : Concern for Authorisation

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR - Agreement concerning the International Carriage of Dangerous Goods by Road

AllC - Australian Inventory of Industrial Chemicals

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

GHS - Globally Harmonized System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Cancer

IATA - International Air Transport Association

IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC50 - Half maximal inhibitory concentration
ICAO - International Civil Aviation Organization
IECSC - Inventory of Existing Chemical Substances in China
IMDG - International Maritime Dangerous Goods
IMO - International Maritime Organization
ISHL - Industrial Safety and Health Law (Japan)
ISO - International Organisation for Standardization
KECI - Korea Existing Chemicals Inventory
LC50 - Lethal Concentration to 50 % of a test population
LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)
MARPOL - International Convention for the Prevention of Pollution from Ships
n.o.s. - Not Otherwise Specified
NO(A)EC - No Observed (Adverse) Effect Concentration
NO(A)EL - No Observed (Adverse) Effect Level
NOELR - No Observable Effect Loading Rate
NZIoC - New Zealand Inventory of Chemicals
OECD - Organization for Economic Co-operation and Development
OPPTS - Office of Chemical Safety and Pollution Prevention
PBT - Persistent, Bioaccumulative and Toxic substance
PICCS - Philippines Inventory of Chemicals and Chemical Substances
(Q)SAR - (Quantitative) Structure Activity Relationship
REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals
RID - Regulations concerning the International Carriage of Dangerous Goods by Rail
SADT - Self-Accelerating Decomposition Temperature
SDS - Safety Data Sheet
TCSI - Taiwan Chemical Substance Inventory
TECI - Thailand Existing Chemicals Inventory
TSCA - Toxic Substances Control Act (United States)
UN - United Nations
UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods
vPvB - Very Persistent and Very Bioaccumulative

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.