

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

1 Identification

- **Product identifier**
- **Trade name:** PHGDH-inactive
- **Synonym**
N-(4,6-dimethyl-2-pyridinyl)-4-(4-pyridinyl)-1-piperazinecarbothioamide
3-Phosphoglycerate Dehydrogenase-inactive
- **Article number:** 19717
- **CAS Number:**
1914971-16-6
- **Application of the substance / the mixture** For research use only - not for human or veterinary use.
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA
- **Information department:** Product safety department
- **Emergency telephone number:**
During normal opening times: +1 (734) 971-3335
US/CANADA: 800-424-9300
Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

- **Classification of the substance or mixture**



GHS07

Skin Irrit. 2 H315 Causes skin irritation.

Aquatic Acute 2 H401 Toxic to aquatic life.

- **Label elements**

- **GHS label elements**

The substance is classified and labeled according to the Globally Harmonized System (GHS).

- **Hazard pictograms**



GHS07

- **Signal word** Warning

- **Hazard statements**

Causes skin irritation.

Toxic to aquatic life.

- **Precautionary statements**

Wash thoroughly after handling.

Avoid release to the environment.

(Contd. on page 2)

US

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

Trade name: PHGDH-inactive

(Contd. from page 1)

Wear protective gloves.
 If on skin: Wash with plenty of water.
 Specific treatment (see on this label).
 If skin irritation occurs: Get medical advice/attention.
 Take off contaminated clothing and wash it before reuse.
 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Classification system:**

- **NFPA ratings (scale 0 - 4)**



Health = 1
 Fire = 0
 Reactivity = 0

- **HMIS-ratings (scale 0 - 4)**



Health = 1
 Fire = 0
 Reactivity = 0

- **Other hazards**
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.

3 Composition/information on ingredients

- **Chemical characterization: Substances**
- **CAS No. Description**
 1914971-16-6 PHGDH-inactive

4 First-aid measures

- **Description of first aid measures**
- **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **After swallowing:** If symptoms persist consult doctor.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed**
 May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects.
 No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**
 No further relevant information available.

5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**
 Use fire fighting measures that suit the environment.
 A solid water stream may be inefficient.
- **Special hazards arising from the substance or mixture** No further relevant information available.

(Contd. on page 3)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

Trade name: PHGDH-inactive

(Contd. from page 2)

- **Advice for firefighters**
- **Protective equipment:** No special measures required.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures** Not required.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:** Pick up mechanically.
- **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
- **Protective Action Criteria for Chemicals**
- **PAC-1:** Substance is not listed.
- **PAC-2:** Substance is not listed.
- **PAC-3:** Substance is not listed.

7 Handling and storage

- **Handling:**
- **Precautions for safe handling**
No special precautions are necessary if used correctly.
Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid prolonged or repeated exposure.
Keep away from sources of ignition.
Take precautionary measures against static discharge.re.
- **Information about protection against explosions and fires:** No special measures required.
- **Conditions for safe storage, including any incompatibilities**
Keep container tightly closed.
Store in accordance with information listed on the product insert.
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** None.
- **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

- **Additional information about design of technical systems:** No further data; see item 7.
- **Control parameters**
- **Components with limit values that require monitoring at the workplace:**
The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.
The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit.
At this time, the remaining constituent has no known exposure limits.
At this time, the other constituents have no known exposure limits.
- **Additional information:** The lists that were valid during the creation were used as basis.

(Contd. on page 4)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

Trade name: PHGDH-inactive

(Contd. from page 3)

- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**
 - Keep away from foodstuffs, beverages and feed.
 - Immediately remove all soiled and contaminated clothing.
 - Wash hands before breaks and at the end of work.
 - Avoid contact with the skin.
 - Avoid contact with the eyes and skin.
- **Breathing equipment:** Not required.
- **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

- **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
- **Eye protection:** Not required.

9 Physical and chemical properties

· Information on basic physical and chemical properties

· General Information

· Appearance:

Form: Crystalline
Color: Not determined.

· **Odor:** Characteristic

· **Structural Formula** C₁₇H₂₁N₅S

· **Molecular Weight** 327.5 g/mol

· **Odor threshold:** Not determined.

· **pH-value:** Not applicable.

· Change in condition

Melting point/Melting range: Undetermined.

Boiling point/Boiling range: Undetermined.

· **Flash point:** Not applicable.

· **Flammability (solid, gaseous):** Product is not flammable.

· **Decomposition temperature:** Not determined.

· **Auto igniting:** Not determined.

· **Danger of explosion:** Product does not present an explosion hazard.

(Contd. on page 5)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

Trade name: PHGDH-inactive

(Contd. from page 4)

· Explosion limits:	
Lower:	Not determined.
Upper:	Not determined.
· Vapor pressure:	Not applicable.
· Density:	Not determined.
· Relative density	Not determined.
· Vapor density	Not applicable.
· Evaporation rate	Not applicable.
· Solubility in / Miscibility with Water:	Not determined.
· Partition coefficient (n-octanol/water):	Not determined.
· Viscosity:	
Dynamic:	Not applicable.
Kinematic:	Not applicable.
SOLUBILITY	~0.16 mg/ml in a 1:15 solution of DMSO:PBS (pH 7.2); ~5 mg/ml in DMSO; ~2 mg/ml in DMF
· Other information	No further relevant information available.

10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** strong oxidizing agents
- **Hazardous decomposition products:** carbon oxides, nitrogen oxides, sulfur oxides

11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**
- **Primary irritant effect:**
- **on the skin:** Irritant to skin and mucous membranes.
- **on the eye:** No irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional toxicological information:**
- **Carcinogenic categories**
- **IARC (International Agency for Research on Cancer)** Substance is not listed.
- **NTP (National Toxicology Program)** Substance is not listed.
- **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.

US

(Contd. on page 6)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

Trade name: PHGDH-inactive

(Contd. from page 5)

12 Ecological information

- **Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **Persistence and degradability** No further relevant information available.
- **Behavior in environmental systems:**
- **Bioaccumulative potential** No further relevant information available.
- **Mobility in soil** No further relevant information available.
- **Additional ecological information:**
- **General notes:**
Water hazard class 1 (Self-assessment): slightly hazardous for water
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Other adverse effects** No further relevant information available.

13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- | | |
|--|-----------------|
| · UN-Number | |
| · DOT, IMDG, IATA | not regulated |
| · UN proper shipping name | |
| · DOT, IMDG, IATA | not regulated |
| · Transport hazard class(es) | |
| · DOT, ADN, IMDG, IATA | |
| · Class | not regulated |
| · Packing group | |
| · DOT, IMDG, IATA | not regulated |
| · Environmental hazards: | Not applicable. |
| · Special precautions for user | Not applicable. |
| · Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code | Not applicable. |
| · UN "Model Regulation": | not regulated |

US

(Contd. on page 7)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

Trade name: PHGDH-inactive

(Contd. from page 6)

15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**
- **Sara**
- **Section 355 (extremely hazardous substances):** Substance is not listed.
- **Section 313 (Specific toxic chemical listings):** Substance is not listed.
- **TSCA (Toxic Substances Control Act):** Substance is not listed.
- **Hazardous Air Pollutants** Substance is not listed.
- **Proposition 65**
- **Chemicals known to cause cancer:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
- **Chemicals known to cause developmental toxicity:** Substance is not listed.
- **Carcinogenic categories**
- **EPA (Environmental Protection Agency)** Substance is not listed.
- **TLV (Threshold Limit Value established by ACGIH)** Substance is not listed.
- **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
- **GHS label elements**
The substance is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



GHS07

- **Signal word** Warning
- **Hazard statements**
Causes skin irritation.
Toxic to aquatic life.
- **Precautionary statements**
Wash thoroughly after handling.
Avoid release to the environment.
Wear protective gloves.
If on skin: Wash with plenty of water.
Specific treatment (see on this label).
If skin irritation occurs: Get medical advice/attention.
Take off contaminated clothing and wash it before reuse.
Dispose of contents/container in accordance with local/regional/national/international regulations.
- **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- **Department issuing SDS:** Environment protection department.
- **Contact:** -
- **Date of preparation / last revision** 09/14/2020 / -
- **Abbreviations and acronyms:**
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
ACGIH: American Conference of Governmental Industrial Hygienists

(Contd. on page 8)

Safety Data Sheet

acc. to OSHA HCS

Printing date 09/14/2020

Revision date 09/14/2020

Trade name: PHGDH-inactive

(Contd. from page 7)

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Skin Irrit. 2: Skin corrosion/irritation – Category 2

Aquatic Acute 2: Hazardous to the aquatic environment - acute aquatic hazard – Category 2

US