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1 Identification

- · Product identifier
- Trade name: PKI-166
- Article number: 21896
- CAS Number: 187724-61-4
- EC number: 808-564-7
- **Application of the substance / the mixture** This product is for research use - Not for human or veterinary diagnostic or therapeutic 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



GHS06 Skull and crossbones

Acute Toxicity - Oral 3 H301 Toxic if swallowed.

- · Label elements
- · GHS label elements

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



· Signal word Danger

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· Hazard statements
H301 Toxic if swallowed.
· Precautionary statements
P264 Wash thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P301+P310 If swallowed: Immediately call a poison center/doctor.
P321 Specific treatment (see on this label).
P330 Rinse mouth.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
· Classification system:
· NFPA ratings (scale 0 - 4)
NFFA Tauliys (Scale V - 4)
Health = 2 Fire = 0 Reactivity = 0
HMIS-ratings (scale 0 - 4)
HEALTH 2 Health = 2
FIRE 0 Fire = 0
REACTIVITY 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
- 187724-61-4 PKI-166
- · Identification number(s)
- EC number: 808-564-7

4 First-aid measures

· Description of first aid measures

• General information:

Immediately remove any clothing soiled by the product.

- In case of irregular breathing or respiratory arrest provide artificial respiration.
- 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. Then consult a doctor.
- After swallowing: Do not induce vomiting; immediately call for medical help.
- · 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.

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• 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.
- 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:

Dispose contaminated material as waste according to item 13.

- 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 Thorough dedusting.
- · Information about protection against explosions and fires: No special measures required.
- · Conditions for safe storage, including any incompatibilities
- Storage: Store in accordance with information listed on the product insert.
- 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: Not required.

Additional information: The lists that were valid during the creation were used as basis.

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· 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.
 Breathing equipment: Not required.
· Protection of hands:
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.

Information on basic physical and chemical properties General Information		
Appearance:		
Form:	Solid	
Color:	Not determined.	
Odor:	Characteristic	
Structural Formula	C20H18N4O	
Molecular Weight	330.4 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.	
Explosion limits:		
Lower:	Not determined.	
Upper:	Not determined.	
Vapor pressure:	Not applicable.	
Density:	Not determined.	

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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	DMSO: soluble	
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 dioxide, carbon monoxide, nitrogen oxides

11 Toxicological information

- · Information on toxicological effects
- · Acute toxicity:
- Primary irritant effect:
- on the skin: No irritant effect.
- 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.

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.

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· 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.

4 Transport information	
· UN-Number · DOT, IMDG, IATA	UN2811
 UN proper shipping name DOT IMDG IATA 	Toxic solids, organic, n.o.s. (PKI-166) TOXIC SOLID, ORGANIC, N.O.S. (PKI-166) Toxic solid, organic, n.o.s. (PKI-166)
· Transport hazard class(es)	
DOT	
TOXIC	
· Class · Label	6.1 Toxic substances 6.1
· IMDG, IATA	
· Class	6.1 Toxic substances
· Label	6.1
 Packing group DOT, IMDG, IATA 	111
· Environmental hazards:	Not applicable.
· Special precautions for user	Warning: Toxic substances
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 Hazard identification number (Kemler code EMS Number: Stowage Category 	e): 60 F-A,S-A A
• Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
· Transport/Additional information:	
DOT Quantity limitations	On passenger aircraft/rail: 100 kg On cargo aircraft only: 200 kg
 IMDG Limited quantities (LQ) Excepted quantities (EQ) 	5 kg Code: E1 Maximum net quantity per inner packaging: 30 g Maximum net quantity per outer packaging: 1000 g
· IATA · Remarks:	When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.
· UN "Model Regulation":	UN 2811 TOXIC SOLID, ORGANIC, N.O.S. (PKI-166), 6.1, III

15 Regulatory information

- Safety, health and environmental regulations/legislation specific for the substance or mixture No further relevant information available.
- · 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) Substance is not listed.
- NIOSH-Ca (National Institute for Occupational Safety and Health) Substance is not listed.
- · Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes (Contd. on page 8)

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no responsibility for incidental or consequential damages, including lost pro these data. It shall be the user's responsibility to develop proper method protection based on the actual conditions of use. While this SDS is based be reliable, Cayman Chemical Company assumes no responsibility for the c the information contained herein.	s of handling and personal on technical data judged to
 Department issuing SDS: Environment protection department. Contact: - Date of preparation / last revision 12/13/2022 Abbreviations and acronyms: IMDG: International Maritime Code for Dangerous Goods DOT: US Department of Transportation IATA: International Air Transport Association EINECS: European Inventory of Existing Commercial Chemical Substances 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 Acute Toxicity - Oral 3: Acute toxicity – Category 3 	