

Safety Data Sheet

acc. to OSHA HCS

Printing date 11/09/2020

Revision date 11/09/2020

1 Identification

- **Product identifier**
- **Trade name:** Pentylenetetrazole
- **Synonym**
 α,β -Cyclopentamethylenetetrazole
1,5-Pentamethylenetetrazole
PTZ
NSC 5729
NSC 66489
6,7,8,9-tetrahydro-5H-etrazolo[1,5-a]azepine
- **Article number:** 18682
- **CAS Number:**
54-95-5
- **EC number:**
200-219-3
- **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**



GHS06 Skull and crossbones

Acute Tox. 3 H301 Toxic if swallowed.



GHS07

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2A H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

- **Label elements**
- **GHS label elements**

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

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- **Hazard pictograms**



GHS06 GHS07

- **Signal word** Danger

- **Hazard statements**

Toxic if swallowed.
 Causes skin irritation.
 Causes serious eye irritation.
 May cause respiratory irritation.

- **Precautionary statements**

Avoid breathing dust/fume/gas/mist/vapors/spray
 Wash thoroughly after handling.
 Do not eat, drink or smoke when using this product.
 Use only outdoors or in a well-ventilated area.
 Wear protective gloves / eye protection / face protection.
 If swallowed: Immediately call a poison center/doctor.
 Specific treatment (see on this label).
 Rinse mouth.
 If on skin: Wash with plenty of water.
 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 Call a poison center/doctor if you feel unwell.
 Take off contaminated clothing and wash it before reuse.
 If skin irritation occurs: Get medical advice/attention.
 If eye irritation persists: Get medical advice/attention.
 Store in a well-ventilated place. Keep container tightly closed.
 Store locked up.
 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Classification system:**

- **NFPA ratings (scale 0 - 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.

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3 Composition/information on ingredients

- **Chemical characterization: Substances**
- **CAS No. Description**
54-95-5 Pentylentetrazole
- **Identification number(s)**
- **EC number: 200-219-3**

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. If symptoms persist, 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.
- **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.
Ensure adequate ventilation.
- **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.

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- **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**
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:** Keep receptacle tightly sealed.
- **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.
- **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 eyes and skin.
- **Breathing equipment:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
- **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.

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· Eye protection:



Tightly sealed goggles

9 Physical and chemical properties

· Information on basic physical and chemical properties

· General Information

· Appearance:

Form:	Crystalline
Color:	Not determined.
Odor:	Characteristic
Structural Formula	C ₆ H ₁₀ N ₄
Molecular Weight	138.2 g/mol
Odor threshold:	Not determined.

· pH-value: Not applicable.

· Change in condition

Melting point/Melting range:	59–61 °C (138.2–141.8 °F)
Boiling point/Boiling range:	194 °C (381.2 °F)

· 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.

· 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 ~3 mg/ml in PBS (pH 7.2); ~30 mg/ml in EtOH; DMSO; DMF

· Other information No further relevant information available.

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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

11 Toxicological information

- **RTECS Number** XF8225000
- **Information on toxicological effects**
- **Acute toxicity:**

- **LD/LC50 values that are relevant for classification:**

Oral	LDLO	147 mg/kg (man)
	LD50	88 mg/kg (mouse) 515 mg/kg (rat)
	Intraperitoneal LD50	55 mg/kg (mouse) 82 mg/kg (rat)
Subcutaneous LD50		70 mg/kg (mouse) 670 mg/kg (rat)

- **Primary irritant effect:**
- **on the skin:** Irritant to skin and mucous membranes.
- **on the eye:** 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.
- **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.

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- **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 | UN2811 |
| · DOT, IMDG, IATA | UN2811 |
| · UN proper shipping name | Toxic solids, organic, n.o.s. (Pentylenetetrazole) |
| · DOT | TOXIC SOLID, ORGANIC, N.O.S. (Pentylenetetrazole) |
| · IMDG | Toxic solid, organic, n.o.s. (Pentylenetetrazole) |
| · IATA | Toxic solid, organic, n.o.s. (Pentylenetetrazole) |
| · Transport hazard class(es) | |
| · DOT | |
| | |
| · Class | 6.1 Toxic substances |
| · Label | 6.1 |
| · IMDG, IATA | |
| | |
| · Class | 6.1 Toxic substances |
| · Label | 6.1 |
| · Packing group | III |
| · DOT, IMDG, IATA | III |
| · Environmental hazards: | Not applicable. |
| · Special precautions for user | Warning: Toxic substances |
| · Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code | Not applicable. |

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<ul style="list-style-type: none"> · Transport/Additional information: · DOT · Quantity limitations <table style="width: 100%; border: none;"> <tr> <td style="width: 40%;"></td> <td>On passenger aircraft/rail: 100 kg</td> </tr> <tr> <td></td> <td>On cargo aircraft only: 200 kg</td> </tr> </table> 			On passenger aircraft/rail: 100 kg		On cargo aircraft only: 200 kg				
	On passenger aircraft/rail: 100 kg								
	On cargo aircraft only: 200 kg								
<ul style="list-style-type: none"> · IMDG · Limited quantities (LQ) <table style="width: 100%; border: none;"> <tr> <td style="width: 40%;"></td> <td>5 kg</td> </tr> </table> · Excepted quantities (EQ) <table style="width: 100%; border: none;"> <tr> <td style="width: 40%;"></td> <td>Code: E1</td> </tr> <tr> <td></td> <td>Maximum net quantity per inner packaging: 30 g</td> </tr> <tr> <td></td> <td>Maximum net quantity per outer packaging: 1000 g</td> </tr> </table> 			5 kg		Code: E1		Maximum net quantity per inner packaging: 30 g		Maximum net quantity per outer packaging: 1000 g
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<ul style="list-style-type: none"> · IATA · Remarks: <table style="width: 100%; border: none;"> <tr> <td style="width: 40%;"></td> <td>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.</td> </tr> </table> 			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.						
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<ul style="list-style-type: none"> · UN "Model Regulation": <table style="width: 100%; border: none;"> <tr> <td style="width: 40%;"></td> <td>UN 2811 TOXIC SOLID, ORGANIC, N.O.S. (PENTYLENETETRAZOLE), 6.1, III</td> </tr> </table> 			UN 2811 TOXIC SOLID, ORGANIC, N.O.S. (PENTYLENETETRAZOLE), 6.1, III						
	UN 2811 TOXIC SOLID, ORGANIC, N.O.S. (PENTYLENETETRAZOLE), 6.1, III								

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):** ACTIVE
- **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.
- **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** 11/09/2020 / -
- **Abbreviations and acronyms:**
 - IMDG: International Maritime Code for Dangerous Goods
 - DOT: US Department of Transportation
 - IATA: International Air Transport Association

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ACGIH: American Conference of Governmental Industrial Hygienists
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)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
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 Tox. 3: Acute toxicity – Category 3
Skin Irrit. 2: Skin corrosion/irritation – Category 2
Eye Irrit. 2A: Serious eye damage/eye irritation – Category 2A
STOT SE 3: Specific target organ toxicity (single exposure) – Category 3

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