Safety Data Sheet
acc. to OSHA HCS

Printing date 03/15/2024 Revision date 03/15/2024

*
1 Identification

· **Product identifier**

· **Trade name: PB-22 8-hydroxyisoquinoline isomer**
· **Synonym** isoquinolin-8-yl 1-pentyl-1H-indole-3-carboxylate

· **Article number:** 14558
· **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

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2 Hazard(s) identification

· **Classification of the substance or mixture**


GHS02 Flame

Flammable Liquids 2	H225 Highly flammable liquid and vapor.


GHS07

Acute Toxicity - Oral 4	H302 Harmful if swallowed.
Acute Toxicity - Dermal 4	H312 Harmful in contact with skin.
Acute Toxicity - Inhalation 4	H332 Harmful if inhaled.
Eye Irritation 2A	H319 Causes serious eye irritation.

· **Label elements**
· **GHS label elements**
The product is classified and labeled according to the Globally Harmonized System (GHS).

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· **Hazard pictograms**

GHS02 GHS07

· **Signal word** Danger

· **Hazard-determining components of labeling:**
Acetonitrile

· **Hazard statements**

H225	Highly flammable liquid and vapor.
H302+H312+H332	Harmful if swallowed, in contact with skin or if inhaled.
H319	Causes serious eye irritation.

· **Precautionary statements**

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ventilating/lighting/equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/fume/gas/mist/vapors/spray
P264	Wash thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P301+P312	If swallowed: Call a poison center/doctor if you feel unwell.
P303+P361+P353	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P321	Specific treatment (see on this label).
P330	Rinse mouth.
P362+P364	Take off contaminated clothing and wash it before reuse.
P337+P313	If eye irritation persists: Get medical advice/attention.
P370+P378	In case of fire: Use CO2, powder or water spray to extinguish.
P403+P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/container in accordance with local/regional/national/international regulations.

· **Classification system:**
· **NFPA ratings (scale 0 - 4)**

Health = 2
Fire = 3
Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**

Health = 2
Fire = 3
Reactivity = 0

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· **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: Mixtures**
· **Description:** Mixture of the substances listed below with nonhazardous additions.

· **Dangerous components:**		
CAS: 75-05-8 RTECS: AL7700000	Acetonitrile	99.0%

· **Other ingredients**		
1798021-82-5	PB-22 8-hydroxyisoquinoline isomer	1.0%

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4 First-aid measures

· **Description of first aid measures**
· **General information:**
Immediately remove any clothing soiled by the product.
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
· **After inhalation:**
Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.
In case of unconsciousness place patient stably in side position for transportation.
· **After skin contact:** Immediately rinse with water.
· **After eye contact:**
Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
· **After swallowing:** Immediately call a doctor.
· **Information for doctor:**
· **Most important symptoms and effects, both acute and delayed**
No further relevant information available.
· **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

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5 Fire-fighting measures

· **Extinguishing media**
· **Suitable extinguishing agents:**
CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
· **Special hazards arising from the substance or mixture**
Can release vapors that form explosive mixtures at temperatures at or above the flashpoint.
Container explosion may occur under fire conditions.
Emits toxic fumes under fire conditions.
Sensitive to static discharge.
Vapors can travel to a source of ignition and flash back.

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· **Advice for firefighters**
· **Protective equipment:** Mouth respiratory protective device.

6 Accidental release measures

· **Personal precautions, protective equipment and emergency procedures**
Wear protective equipment. Keep unprotected persons away.
· **Environmental precautions:**
Dilute with plenty of water.
Do not allow to enter sewers/ surface or ground water.
· **Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose contaminated material as waste according to section 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:**		
75-05-8	Acetonitrile	13 ppm
· **PAC-2:**		
75-05-8	Acetonitrile	50 ppm
· **PAC-3:**		
75-05-8	Acetonitrile	150 ppm

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7 Handling and storage

· **Handling:**
· **Precautions for safe handling**
Ensure good ventilation/exhaustion at the workplace.
Prevent formation of aerosols.
· **Information about protection against explosions and fires:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.

· **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:** Store in a cool location.
· **Information about storage in one common storage facility:** Not required.
· **Further information about storage conditions:**
Keep receptacle tightly sealed.
Store in cool, dry conditions in well sealed receptacles.
· **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 section 7.

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· **Control parameters**

· **Components with limit values that require monitoring at the workplace:**	
75-05-8 Acetonitrile	
PEL	Long-term value: 70 mg/m³, 40 ppm
REL	Long-term value: 34 mg/m³, 20 ppm
TLV	Long-term value: 20 ppm Skin, A4

· **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.
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. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.
· **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:**

Tightly sealed goggles

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9 Physical and chemical properties

· **Information on basic physical and chemical properties**
· **General Information**
· **Appearance:**
Form: Liquid

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Color:	According to product specification
· **Odor:**	Characteristic
· **Structural Formula**	C23H22N2O2
· **Molecular Weight**	358.4 g/mol
· **Odor threshold:**	Not determined.
· **Formulation**	A solution in acetonitrile
· **pH-value:**	Not determined.
· **Change in condition**	
Melting point/Melting range:	-46 °C (-50.8 °F)
Boiling point/Boiling range:	81 °C (177.8 °F)
· **Flash point:**	2 °C (35.6 °F)
· **Flammability (solid, gaseous):**	Highly flammable.
· **Auto igniting:**	525 °C (977 °F)
· **Decomposition temperature:**	Not determined.
· **Ignition temperature:**	Product is not selfigniting.
· **Danger of explosion:**	Product is not explosive. However, formation of explosive air/ vapor mixtures are possible.
· **Explosion limits:**	
Lower:	4.4 Vol %
Upper:	16 Vol %
· **Vapor pressure at 20 °C (68 °F):**	98.64 hPa (74 mm Hg)
· **Vapor pressure at 50 °C (122 °F):**	330 hPa (247.5 mm Hg)
· **Density at 20 °C (68 °F):**	0.79 g/cm³ (6.59255 lbs/gal)
· **Relative density**	Not determined.
· **Vapor density**	Not determined.
· **Evaporation rate**	Not determined.
· **Solubility in / Miscibility with**	
Water at 25 °C (77 °F):	1000 g/l
· **Partition coefficient (n-octanol/water):**	Not determined.
· **Viscosity:**	
Dynamic at 20 °C (68 °F):	0.35 mPas
Kinematic:	Not determined.
SOLUBILITY	DMF: 11 mg/ml, DMF:PBS(pH 7.2)(1:1): 0.33 mg/ml, DMSO: 10 mg/ml
· **Solvent content:**	
VOC content:	0.00 % 0.0 g/l / 0.00 lb/gal
Solids content:	1.0 %
· **Other information**	No further relevant information available.

10 Stability and reactivity

· **Reactivity** No further relevant information available.

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· **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, alkali metals, acids, bases, reducing agents
· **Hazardous decomposition products:**
carbon dioxide, carbon monoxide, hydrogen cyanide, nitrogen oxides

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11 Toxicological information

· **Information on toxicological effects**
· **Acute toxicity:**

· **LD/LC50 values that are relevant for classification:**		
ATE (Acute Toxicity Estimate)		
Oral	LD50	623 mg/kg (mouse)
Dermal	LD50	1,515 mg/kg (rabbit)
Inhalative	LC50/4 h	11.1 mg/l

75-05-8 Acetonitrile		
Oral	LD50	617 mg/kg (mouse) (OECD Test Guideline 401)
Dermal	LD50	1,500 mg/kg (rabbit) (Expert Judgement) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Inhalative	LC50/4 h	6.022 mg/l (mouse) (OECD Test Guideline 403)

· **Primary irritant effect:**
· **on the skin:** No irritant effect.
· **on the eye:** Irritating effect.
· **Sensitization:** No sensitizing effects known.
· **Additional toxicological information:**
The product shows the following dangers according to internally approved calculation methods for preparations:
Harmful
Irritant

· **Carcinogenic categories**

· **IARC (International Agency for Research on Cancer)**
None of the ingredients is listed.

· **NTP (National Toxicology Program)**
None of the ingredients is listed.

· **OSHA-Ca (Occupational Safety & Health Administration)**
None of the ingredients is listed.

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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 2 (Self-assessment): hazardous for water
Do not allow product to reach ground water, water course or sewage system.
Danger to drinking water if even small quantities leak into the ground.
· **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.
· **Recommended cleansing agent:** Water, if necessary with cleansing agents.

14 Transport information

· **UN-Number**	
· **DOT, IMDG, IATA**	UN1648
· **UN proper shipping name**	
· **DOT, IATA**	Acetonitrile solution
· **IMDG**	ACETONITRILE solution
· **Transport hazard class(es)**	
· **DOT**	

· **Class**	3 Flammable liquids
· **Label**	3

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· **IMDG, IATA**

· **Class**	3 Flammable liquids
· **Label**	3
· **Packing group**	
· **DOT, IMDG, IATA**	II
· **Environmental hazards:**	Not applicable.
· **Special precautions for user**	Warning: Flammable liquids
· **Hazard identification number (Kemler code):**	33
· **EMS Number:**	F-E,S-D
· **Stowage Category**	B
· **Stowage Code**	SW2 Clear of living quarters.
· **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: 5 L On cargo aircraft only: 60 L
· **IMDG**	
· **Limited quantities (LQ)**	1L
· **Excepted quantities (EQ)**	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· **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 1648 ACETONITRILE SOLUTION, 3, II

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):**

None of the ingredients is listed.

· **Section 313 (Specific toxic chemical listings):**

75-05-8	Acetonitrile

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· **TSCA (Toxic Substances Control Act):**

75-05-8	Acetonitrile	ACTIVE

· **Hazardous Air Pollutants**

75-05-8	Acetonitrile

· **Proposition 65**

· **Chemicals known to cause cancer:**

None of the ingredients is listed.

· **Chemicals known to cause reproductive toxicity for females:**

None of the ingredients is listed.

· **Chemicals known to cause reproductive toxicity for males:**

None of the ingredients is listed.

· **Chemicals known to cause developmental toxicity:**

None of the ingredients is listed.

· **Carcinogenic categories**

· **EPA (Environmental Protection Agency)**

75-05-8	Acetonitrile	CBD, D

· **TLV (Threshold Limit Value)**

75-05-8	Acetonitrile	A4

· **NIOSH-Ca (National Institute for Occupational Safety and Health)**

None of the ingredients is 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 no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

· **Department issuing SDS:** Environment protection department.
· **Contact:** -
· **Date of preparation / last revision** 03/15/2024 / -
· **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
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
VOC: Volatile Organic Compounds (USA, EU)
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

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TLV: Threshold Limit Value
PEL: Permissible Exposure Limit
REL: Recommended Exposure Limit
Flammable Liquids 2: Flammable liquids – Category 2
Acute Toxicity - Oral 4: Acute toxicity – Category 4
Eye Irritation 2A: Serious eye damage/eye irritation – Category 2A

· *** Data compared to the previous version altered.**