

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 1272/2008

**Section 1. Identification of the Substance/Mixture and of the Company/Undertaking**

- 1.1 Product Code:** 22871  
**Product Name:** PB-22-d9 (exempt preparation)  
**Synonyms:** 1-pentyl-2,2',3,3',4,4',5,5,5-d9-8-quinolinyl ester-1H-indole-3-carboxylic acid; QUPIC-d9;
- 1.2 Relevant identified uses of the substance or mixture and uses advised against:**  
**Relevant identified uses:** For research use only, not for human or veterinary use.
- 1.3 Details of the Supplier of the Safety Data Sheet:**  
**Company Name:** Cayman Chemical Company  
1180 E. Ellsworth Rd.  
Ann Arbor, MI 48108  
**Web site address:** www.caymanchem.com  
**Information:** Cayman Chemical Company +1 (734)971-3335
- 1.4 Emergency telephone number:**  
**Emergency Contact:** CHEMTREC Within USA and Canada: +1 (800)424-9300  
CHEMTREC Outside USA and Canada: +1 (703)527-3887

**Section 2. Hazards Identification**

- 2.1 Classification of the Substance or Mixture:**  
**Flammable Liquids, Category 2**  
**Acute Toxicity: Inhalation, Category 4**  
**Acute Toxicity: Oral, Category 4**  
**Acute Toxicity: Skin, Category 4**  
**Serious Eye Damage/Eye Irritation, Category 2**

**2.2 Label Elements:****GHS Signal Word:** **Danger****GHS Hazard Phrases:**

H225: Highly flammable liquid and vapor.

H302: Harmful if swallowed.

H312: Harmful in contact with skin.

H319: Causes serious eye irritation.

H332: Harmful if inhaled.

**GHS Precaution Phrases:**

P210: Keep away from {heat/sparks/open flames/hot surfaces}. - No smoking.

P261: Avoid breathing {dust/fume/gas/mist/vapors/spray}.

P264: Wash {hands} thoroughly after handling.

P280: Wear {protective gloves/protective clothing/eye protection/face protection}.

**GHS Response Phrases:**

P301+312: IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.

P302+352: IF ON SKIN: Wash with plenty of soap and water.

P303+361+353: IF ON SKIN (or hair): Remove/take off immediately all contaminated clothing. Rinse skin with water/shower.

P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P305+351+338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy

to do. Continue rinsing.  
 P312: Call a POISON CENTER or doctor/physician if you feel unwell.  
 P330: Rinse mouth.  
 P337+313: If eye irritation persists, get medical advice/attention.  
 P362+364: Take off contaminated clothing and wash it before reuse.

**GHS Storage and Disposal Phrases:**

Please refer to Section 7 for Storage and Section 13 for Disposal information.

**2.3 Adverse Human Health** Can cause fatal cyanide poisoning.  
**Effects and Symptoms:** Causes serious eye irritation.  
 Harmful if swallowed, inhaled, or absorbed through the skin.  
 Material may be irritating to the mucous membranes and upper respiratory tract.  
 May be fatal if swallowed, inhaled, or absorbed through the skin.  
 May cause skin or respiratory system irritation.  
 Several hours may elapse from exposure to onset of symptoms.  
 To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

**Section 3. Composition/Information on Ingredients**

CAS # / RTECS #	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	GHS Classification
NA NA	PB-22-d9	0.1 %	NA NA	No data available.
75-05-8 AL7700000	Acetonitrile	99.9 %	200-835-2 608-001-00-3	Flam. Liq. 2: H225 Acute Tox.(O) 4: H302 Acute Tox.(D) 4: H312 Eye Damage 2: H319 Acute Tox.(I) 4: H332

**Section 4. First Aid Measures**

**4.1 Description of First Aid Measures:**

**In Case of Inhalation:** Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.

**In Case of Skin Contact:** Immediately wash skin with soap and plenty of water for at least 15 minutes. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

**In Case of Eye Contact:** Hold eyelids apart and flush eyes with plenty of water for at least 15 minutes. Have eyes examined and tested by medical personnel.

**In Case of Ingestion:** Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.

**4.2 Important Symptoms and Effects, Both Acute and Delayed:** Exposure may cause: asphyxia, cyanosis, depression, diarrhea, dizziness, drowsiness, excitement, headache, impaired judgement, lack of coordination, nausea, rash, vomiting, stupor, death.  
 Treat as cyanide poisoning. Always have on hand a cyanide first-aid kit, together with proper instructions. The onset of symptoms is generally delayed pending conversion to cyanide.

**Note for the Doctor:** Acetonitrile is metabolized to cyanide. Patients with significant exposures must be observed for signs of cyanide poisoning and treated accordingly.

### Section 5. Fire Fighting Measures

- 5.1 Suitable Extinguishing** Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.  
**Media:** Use water spray to cool fire-exposed containers.  
**Unsuitable Extinguishing** A solid water stream may be inefficient.  
**Media:**
- 5.2 Flammable Properties and Hazards:** 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.  
 No data available.  
**Flash Pt:** 2.00 C Method Used: Closed Cup  
**Explosive Limits:** LEL: 3.0% at 25.0 C UEL: 16.0% at 25.0 C  
**Autoignition Pt:** 524.00 C
- 5.3 Fire Fighting Instructions:** As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.  
 Note: Flammable as diluted in acetonitrile.

### Section 6. Accidental Release Measures

- 6.1 Protective Precautions,** Avoid breathing vapors and provide adequate ventilation.  
**Protective Equipment and Emergency Procedures:** As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator, and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
- 6.2 Environmental Precautions:** Take steps to avoid release into the environment, if safe to do so.
- 6.3 Methods and Material For Containment and Cleaning Up:** Contain spill and collect, as appropriate.  
 Transfer to a chemical waste container for disposal in accordance with local regulations.

### Section 7. Handling and Storage

- 7.1 Precautions To Be Taken in Handling:** 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.
- 7.2 Precautions To Be Taken in Storing:** Keep away from heat, sparks and flame.  
 Keep container tightly closed.  
 Store in accordance with information listed on the product insert.

### Section 8. Exposure Controls/Personal Protection

**8.1 Exposure Parameters:**

CAS #	Chemical Name	Jurisdiction	Recommended Exposure Limits	Notations
75-05-8	Acetonitrile	ACGIH TLV	TLV: 20 ppm	
		Europe	TWA: 70 mg/m3 (40 ppm)	Skin Absorption
		France VL	TWA: 70 mg/m3 (40 ppm) STEL: ()	
		OSHA PELs	PEL: 40 ppm	
		Britain EH40	TWA: 68 mg/m3 (40 ppm) STEL: 102 mg/m3 (60 ppm)	

**8.2 Exposure Controls:**

**8.2.1 Engineering Controls (Ventilation etc.):** Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.

**8.2.2 Personal protection equipment:**

**Eye Protection:** Safety glasses

**Protective Gloves:** Compatible chemical-resistant gloves

**Other Protective Clothing:** Lab coat

**Respiratory Equipment (Specify Type):** NIOSH approved respirator, as conditions warrant.

**Work/Hygienic/Maintenance Practices:** Do not take internally.

Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower.

Wash thoroughly after handling.

No data available.

**Section 9. Physical and Chemical Properties**

**9.1 Information on Basic Physical and Chemical Properties**

**Physical States:** [ ] Gas [X] Liquid [ ] Solid

**Appearance and Odor:** A 1 mg/ml solution in acetonitrile

**pH:** No data.

**Melting Point:** No data.

**Boiling Point:** No data.

**Flash Pt:** 2.00 C Method Used: Closed Cup

**Evaporation Rate:** No data.

**Flammability (solid, gas):** No data available.

**Explosive Limits:** LEL: 3.0% at 25.0 C UEL: 16.0% at 25.0 C

**Vapor Pressure (vs. Air or mm Hg):** 73 MM\_HG at 20.0 C

**Vapor Density (vs. Air = 1):** No data.

**Specific Gravity (Water = 1):** No data.

**Solubility in Water:** No data.

**Octanol/Water Partition Coefficient:** No data.

**Autoignition Pt:** 524.00 C

**Decomposition Temperature:** No data.

**Viscosity:** No data.

**9.2 Other Information**

**Percent Volatile:** No data.

**Molecular Formula & Weight:** C23H13D9N2O2 367.5

### Section 10. Stability and Reactivity

- 10.1 Reactivity:** No data available.
- 10.2 Stability:** Unstable [ ] Stable [ X ]
- 10.3 Stability Note(s):** Stable if stored in accordance with information listed on the product insert.
- Polymerization:** Will occur [ ] Will not occur [ X ]
- 10.4 Conditions To Avoid:** heat, flames and sparks
- 10.5 Incompatibility - Materials To Avoid:** acids  
alkali metals  
bases  
oxidizing agents  
reducing agents
- 10.6 Hazardous Decomposition or Byproducts:** carbon dioxide  
carbon monoxide  
hydrogen cyanide  
nitrogen oxides

### Section 11. Toxicological Information

- 11.1 Information on Toxicological Effects:** The toxicological effects of this product have not been thoroughly studied.  
Acetonitrile - Toxicity Data: Oral LD50 (rat): 2,460 mg/kg; Oral LD50 (mouse): 269 mg/kg; Oral LD50 (rabbit): 50 mg/kg; Oral TDLO (man): 64 mg/kg; Skin LD50 (rabbit): 980 mg/kg; Inhalation TCLO (human): 160 ppm (4h); Inhalation LC50 (rat): 7,551 ppm (8h);  
Acetonitrile - Irritation Data: Skin (rabbit) 500 mg mild; Eye (rabbit): 100 µl (24 hr) moderate;
- Chronic Toxicological Effects:** Acetonitrile - Investigated as a mutagen, reproductive effector, and tumorigen.  
Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here.  
See actual entry in RTECS for complete information.  
Acetonitrile RTECS Number: AL7700000
- Carcinogenicity:** NTP? No IARC Monographs? No OSHA Regulated? No

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
NA	PB-22-d9	n.a.	n.a.	n.a.	n.a.
75-05-8	Acetonitrile	n.a.	n.a.	A4	n.a.

### Section 12. Ecological Information

- 12.1 Toxicity:** Avoid release into the environment.  
Runoff from fire control or dilution water may cause pollution.
- 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:** No data available.
- 12.6 Other adverse effects:** No data available.

### Section 13. Disposal Considerations

**13.1 Waste Disposal Method:** Dispose in accordance with local, state, and federal regulations.

### Section 14. Transport Information

**14.1 LAND TRANSPORT (US DOT):**

**DOT Proper Shipping Name:** Acetonitrile Solution  
**DOT Hazard Class:** 3 FLAMMABLE LIQUID  
**UN/NA Number:** 1648 **Packing Group:** II



**14.1 LAND TRANSPORT (European ADR/RID):**

**ADR/RID Shipping Name:** Acetonitrile Solution  
**UN Number:** 1648 **Packing Group:** II  
**Hazard Class:** 3 - FLAMMABLE LIQUID

**14.3 AIR TRANSPORT (ICAO/IATA):**

**ICAO/IATA Shipping Name:** Acetonitrile Solution  
**UN Number:** 1648 **Packing Group:** II  
**Hazard Class:** 3 - FLAMMABLE LIQUID **IATA Classification:** 3

**Additional Transport Information:** Transport in accordance with local, state, and federal regulations.  
 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.

### Section 15. Regulatory Information

**EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists**

CAS #	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
NA	PB-22-d9	No	No	No
75-05-8	Acetonitrile	No	Yes 5000 LB	Yes

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
NA	PB-22-d9	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No
75-05-8	Acetonitrile	CAA HAP,ODC: HAP; CWA NPDES: No; TSCA: Yes - Inventory, 8A PAIR; CA PROP.65: No

**Regulatory Information Statement:** This SDS was prepared in accordance with 29 CFR 1910.1200 and Regulation (EC) No.1272/2008.

## Section 16. Other Information

**Revision Date:** 09/23/2017

**Additional Information About** No data available.

**This Product:**

**Company Policy or Disclaimer:** DISCLAIMER: This information is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.