

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 2015/830 and US OSHA HCS 2015

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

- 1.1 Product Code:** 17197
Product Name: 5-PAHSA-d31
Synonyms: 5-(palmitoyloxy-2,2',3,3',4,4',5,5',6,6',7,7',8,8',9,9',10,10',11,11',12,12',13,13',14,14',15,15',16,16,16-d31) octadecanoic acid;
- 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
Serious Eye Damage/Eye Irritation, Category 2
Specific Target Organ Toxicity (single exposure), Category 3

2.2 Label Elements:



GHS Signal Word: **Danger**

GHS Hazard Phrases:

EUH066: Repeated exposure may cause skin dryness or cracking.

H225: Highly flammable liquid and vapor.

H319: Causes serious eye irritation.

H336: May cause drowsiness or dizziness.

GHS Precaution Phrases:

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

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

P264: Wash {hands} thoroughly after handling.

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

GHS Response Phrases:

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.

P337+313: If eye irritation persists, get medical advice/attention.

GHS Storage and Disposal Phrases:

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

2.3 Adverse Human Health Causes serious eye irritation.
Effects and Symptoms: Material may be irritating to the mucous membranes and upper respiratory tract.
 May be harmful by inhalation, ingestion, or skin absorption.
 May cause drowsiness or dizziness.
 May cause skin or respiratory system irritation.
 Repeated exposure may cause skin dryness or cracking.
 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	5-PAHSA-d31	0.1 %	NA NA	No data available.
79-20-9 AI9100000	Methyl acetate 01-2119459211-47	99.9 %	201-185-2 607-021-00-X	Flam. Liq. 2: H225 Eye Damage 2: H319 STOT (SE) 3: H335 H336 EUH066

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: coughing, dizziness, drowsiness, headache, narcosis, optic nerve atrophy, chest tightness.

Section 5. Fire Fighting Measures

5.1 Suitable Extinguishing Media: Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.
Media: Use water spray to cool fire-exposed containers.
Unsuitable Extinguishing Media: A solid water stream may be inefficient.

5.2 Flammable Properties and Hazards: Can release vapors that form explosive mixtures at temperatures at or above the flash point.
 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: -10.00 C Method Used: Closed Cup

Explosive Limits: LEL: 3.1% at 25.0 C UEL: 16.0% at 25.0 C

Autoignition Pt: 455.00 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 methyl acetate.

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.

Other Precautions: Protect from moisture.

Section 8. Exposure Controls/Personal Protection

8.1 Exposure Parameters:

CAS #	Chemical Name	Jurisdiction	Recommended Exposure Limits	Notations
79-20-9	Methyl acetate	ACGIH TLV	TLV: 200 ppm STEL: 250 ppm	
		France VL	TWA: 610 mg/m3 (200 ppm) STEL: 760 mg/m3 (250 ppm)	
		OSHA PELs	PEL: 200 ppm	
		Britain EH40	TWA: 616 mg/m3 (200 ppm) STEL: 770 mg/m3 (250 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 solution in methyl acetate

pH: No data.

Melting Point: No data.

Boiling Point: No data.

Flash Pt: -10.00 C Method Used: Closed Cup

Evaporation Rate: No data.

Flammability (solid, gas): No data available.

Explosive Limits: LEL: 3.1% at 25.0 C UEL: 16.0% at 25.0 C

Vapor Pressure (vs. Air or mm Hg): 173 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: 455.00 C

Decomposition Temperature: No data.

Viscosity: No data.

9.2 Other Information

Percent Volatile: No data.

Molecular Formula & Weight: C34H35D31O4 570.1

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
alkalis
nitrates
strong oxidizing agents

10.6 Hazardous Decomposition or Byproducts: carbon dioxide
carbon monoxide

Section 11. Toxicological Information

11.1 Information on Toxicological Effects: The toxicological effects of this product have not been thoroughly studied.
Methyl Acetate - Toxicity Data: Oral LD50 (rat): >5,000 mg/kg; Oral LD50 (rabbit): 3,705 mg/kg; Skin LD50 (rabbit): >5,000 mg/kg; Inhalation TCLO (human): 15,000 mg/m³;
Methyl Acetate - Irritation Data: Skin (rabbit): 500 mg (24h) mild; Eyes (rabbit): 100 mg (24h) moderate;

Chronic Toxicological Effects: Methyl acetate - Investigated as a mutagen and primary irritant.
Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here.
See actual entry in RTECS for complete information.
Methyl Acetate RTECS Number: AI9100000

Carcinogenicity: NTP? No IARC Monographs? No OSHA Regulated? No

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
NA	5-PAHSA-d31	n.a.	n.a.	n.a.	n.a.
79-20-9	Methyl acetate	n.a.	n.a.	n.a.	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: Methyl Acetate Solution
DOT Hazard Class: 3 FLAMMABLE LIQUID
UN/NA Number: UN1231 **Packing Group:** II



14.1 LAND TRANSPORT (European ADR/RID):

ADR/RID Shipping Name: Methyl Acetate Solution
UN Number: 1231 **Packing Group:** II
Hazard Class: 3 - FLAMMABLE LIQUID

14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Methyl Acetate Solution
UN Number: 1231 **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	5-PAHSA-d31	No	No	No
79-20-9	Methyl acetate	No	No	No

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
NA	5-PAHSA-d31	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No
79-20-9	Methyl acetate	CAA HAP,ODC: No; 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: 09/04/2018

Additional Information About This Product: No data available.

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.