

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

## 1 Identification

- **Product identifier**
- **Trade name: 9-PAHSA-d4**
- **Synonym** 9-[(1-oxohexadecyl)oxy-7,7',8,?8'-d4]-octadecanoic acid
- **Article number:** 17724, 013883
- **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**



GHS02 Flame

Flam. Liq. 2 H225 Highly flammable liquid and vapor.



GHS07

Eye Irrit. 2A H319 Causes serious eye irritation.

STOT SE 3 H336 May cause drowsiness or dizziness.

- **Label elements**

- **GHS label elements**

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

- **Hazard pictograms**



GHS02 GHS07

- **Signal word** Danger

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

Methyl acetate

- **Hazard statements**

H225 Highly flammable liquid and vapor.

H319 Causes serious eye irritation.

(Contd. on page 2)

US

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 1)

H336 May cause drowsiness or dizziness.

· **Precautionary statements**

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Ground/bond container and receiving equipment.

Use explosion-proof electrical/ventilating/lighting/equipment.

Use only non-sparking tools.

Take precautionary measures against static discharge.

Avoid breathing dust/fume/gas/mist/vapors/spray

Wash thoroughly after handling.

Use only outdoors or in a well-ventilated area.

Wear protective gloves/protective clothing/eye protection/face protection.

If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

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.

If eye irritation persists: Get medical advice/attention.

In case of fire: Use for extinction: CO<sub>2</sub>, powder or water spray.

Store in a well-ventilated place. Keep container tightly closed.

Store in a well-ventilated place. Keep cool.

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 = 3

Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**



Health = 2

Fire = 3

Reactivity = 0

· **Other hazards**

· **Results of PBT and vPvB assessment**

· **PBT:** Not applicable.

· **vPvB:** Not applicable.

## 3 Composition/information on ingredients

· **Chemical characterization: Mixtures**

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

· **Dangerous components:**

|                            |                |       |
|----------------------------|----------------|-------|
| CAS: 79-20-9               | Methyl acetate | 99.9% |
| RTECS: AI9100000           |                |       |
| · <b>Other ingredients</b> |                |       |
| 9-PAHSA-d4                 |                | 0.1%  |

US

(Contd. on page 3)

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 2)

## 4 First-aid measures

- **Description of first aid measures**
- **General information:** Immediately remove any clothing soiled by the product.
- **After inhalation:** Supply fresh air; consult doctor in case of complaints.
- **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:** If symptoms persist consult doctor.
- **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:**  
CO<sub>2</sub>, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **For safety reasons unsuitable extinguishing agents:** Water with full jet
- **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.
- **Advice for firefighters**
- **Protective equipment:** No special measures required.

## 6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**  
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:** 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 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:**

|         |                |         |
|---------|----------------|---------|
| 79-20-9 | Methyl acetate | 250 ppm |
|---------|----------------|---------|

- **PAC-2:**

|         |                |           |
|---------|----------------|-----------|
| 79-20-9 | Methyl acetate | 1,700 ppm |
|---------|----------------|-----------|

(Contd. on page 4)

US

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 3)

· **PAC-3:**

79-20-9 Methyl acetate

10000\* ppm

## 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**  
Keep container tightly closed.  
Store in accordance with information listed on the product insert.
- **Storage:**
- **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 item 7.
- **Control parameters**

· **Components with limit values that require monitoring at the workplace:****79-20-9 Methyl acetate**

|     |   |
|-----|---|
| PEL | Long-term value: 610 mg/m <sup>3</sup> , 200 ppm  |
| REL | Short-term value: 760 mg/m <sup>3</sup> , 250 ppm<br>Long-term value: 610 mg/m <sup>3</sup> , 200 ppm |
| TLV | Short-term value: 757 mg/m <sup>3</sup> , 250 ppm<br>Long-term value: 606 mg/m <sup>3</sup> , 200 ppm |

- **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.

(Contd. on page 5)

US

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 4)

- **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

## 9 Physical and chemical properties

- **Information on basic physical and chemical properties**

- **General Information**

- **Appearance:**

Form:

Liquid

Color:

According to product specification

- **Odor:**

Characteristic

- **Structural Formula**

C34H62D4O4

- **Molecular Weight**

542.9

- **Odor threshold:**

Not determined.

- **Formulation**

A solution in methyl acetate

- **pH-value:**

Not determined.

- **Change in condition**

Melting point/Melting range:

-98.05 °C (-144.5 °F)

Boiling point/Boiling range:

Undetermined.

- **Flash point:**

-13 °C (8.6 °F)

- **Flammability (solid, gaseous):**

Not applicable.

- **Ignition temperature:**

455 °C (851 °F)

- **Decomposition temperature:**

Not determined.

- **Auto igniting:**

Product is not selfigniting.

- **Danger of explosion:**

Product is not explosive. However, formation of explosive air/ vapor mixtures are possible.

(Contd. on page 6)

US

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 5)

|   |  |
|---|--|
| · <b>Explosion limits:</b>  |  |
| <b>Lower:</b>   | 3.1 Vol %                                  |
| <b>Upper:</b>   | 16 Vol %                                   |
| · <b>Vapor pressure at 20 °C (68 °F):</b>                         | 220 hPa (165 mm Hg)                        |
| · <b>Density at 20 °C (68 °F):</b>                                | 0.93 g/cm <sup>3</sup> (7.76085 lbs/gal)   |
| · <b>Bulk density:</b>  | 1 kg/m <sup>3</sup>                        |
| · <b>Relative density</b>   | Not determined.                            |
| · <b>Vapor density</b>  | Not determined.                            |
| · <b>Evaporation rate</b>   | Not determined.                            |
| · <b>Solubility in / Miscibility with Water at 20 °C (68 °F):</b> | 330 g/l                                    |
| · <b>Partition coefficient (n-octanol/water):</b>                 | Not determined.                            |
| · <b>Viscosity:</b>   |  |
| <b>Dynamic:</b>   | Not determined.                            |
| <b>Kinematic:</b>   | Not determined.                            |
| · <b>Solvent content:</b>   |  |
| <b>Organic solvents:</b>  | 99.9 %                                     |
| <b>VOC content:</b>   | 0.00 %<br>0.0 g/l / 0.00 lb/gal            |
| · <b>Other information</b>  | 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:** No further relevant information available.
- **Hazardous decomposition products:** No dangerous decomposition products known.

## 11 Toxicological information

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

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

### ATE (Acute Toxicity Estimate)

|      |      |                      |
|------|------|----------------------|
| Oral | LD50 | 3,709 mg/kg (rabbit) |
|------|------|----------------------|

### 79-20-9 Methyl acetate

|            |      |  |
|------------|------|--|
| Oral       | LD50 | >5,000 mg/kg (rat)<br>3,705 mg/kg (rabbit) |
| Dermal     | LD50 | >5,000 mg/kg (rabbit)                      |
| Inhalative | TCLO | 15,000 mg/m <sup>3</sup> (hmn)             |

(Contd. on page 7)

# Safety Data Sheet

## acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 6)

|                    |                      |                       |
|--------------------|----------------------|-----------------------|
| Irritation of skin | Irritation           | 500 mg/24h (rabbit)   |
|                    | Irritation           | 40 mg/kg/24h (rabbit) |
| Irritation of eyes | Irritation           | 100 mg/24h (rabbit)   |
|                    | Intraperitoneal LD50 | 70 mg/kg (mouse)      |

- **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:

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.

## 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.

- **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.

(Contd. on page 8)

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020



Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 7)

- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

## 14 Transport information

|  |  |
|--|--|
| <ul style="list-style-type: none"> <li>· <b>UN-Number</b></li> <li>· <b>DOT, IMDG, IATA</b></li> </ul>   | UN1231   |
| <ul style="list-style-type: none"> <li>· <b>UN proper shipping name</b></li> <li>· <b>DOT, IATA</b></li> <li>· <b>IMDG</b></li> </ul>  | Methyl acetate solution<br>METHYL ACETATE solution   |
| <ul style="list-style-type: none"> <li>· <b>Transport hazard class(es)</b></li> <li>· <b>DOT</b></li> </ul>  | <div style="text-align: center;">  <p>3</p> </div>  |
| <ul style="list-style-type: none"> <li>· <b>Class</b></li> <li>· <b>Label</b></li> </ul>   | 3 Flammable liquids<br>3   |
| <ul style="list-style-type: none"> <li>· <b>IMDG, IATA</b></li> </ul>  | <div style="text-align: center;">  <p>3</p> </div> |
| <ul style="list-style-type: none"> <li>· <b>Class</b></li> <li>· <b>Label</b></li> </ul>   | 3 Flammable liquids<br>3   |
| <ul style="list-style-type: none"> <li>· <b>Packing group</b></li> <li>· <b>DOT, IMDG, IATA</b></li> </ul>   | II   |
| <ul style="list-style-type: none"> <li>· <b>Environmental hazards:</b></li> </ul>  | Not applicable.  |
| <ul style="list-style-type: none"> <li>· <b>Special precautions for user</b></li> <li>· <b>Hazard identification number (Kemler code):</b></li> <li>· <b>EMS Number:</b></li> <li>· <b>Stowage Category</b></li> </ul> | Warning: Flammable liquids<br>33<br>F-E,S-D<br>B   |
| <ul style="list-style-type: none"> <li>· <b>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b></li> </ul>   | Not applicable.  |
| <ul style="list-style-type: none"> <li>· <b>Transport/Additional information:</b></li> <li>· <b>DOT</b></li> <li>· <b>Quantity limitations</b></li> </ul>  | On passenger aircraft/rail: 5 L<br>On cargo aircraft only: 60 L  |
| <ul style="list-style-type: none"> <li>· <b>IMDG</b></li> <li>· <b>Limited quantities (LQ)</b></li> <li>· <b>Excepted quantities (EQ)</b></li> </ul>   | 1L<br>Code: E2<br>Maximum net quantity per inner packaging: 30 ml<br>Maximum net quantity per outer packaging: 500 ml                |

(Contd. on page 9)

US



# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

Trade name: 9-PAHSA-d4

(Contd. from page 8)

- |  |  |
|--|--|
| <ul style="list-style-type: none"> <li>· <b>IATA</b></li> <li>· <b>Remarks:</b></li> </ul> | <p>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.</p> |
| <ul style="list-style-type: none"> <li>· <b>UN "Model Regulation":</b></li> </ul>          | <p>UN 1231 METHYL ACETATE SOLUTION, 3, II</p>  |

## 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):**

None of the ingredients is listed.

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

79-20-9 Methyl acetate

ACTIVE

- **Hazardous Air Pollutants**

None of the ingredients is listed.

- **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)**

None of the ingredients is listed.

- **TLV (Threshold Limit Value established by ACGIH)**

None of the ingredients is listed.

- **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

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.

(Contd. on page 10)

# Safety Data Sheet

acc. to OSHA HCS

Printing date 11/27/2020

Revision date 11/27/2020

**Trade name: 9-PAHSA-d4**

(Contd. from page 9)

- **Department issuing SDS:** Environment protection department.
- **Contact:** -
- **Date of preparation / last revision** 11/27/2020 / -
- **Abbreviations and acronyms:**
  - IMDG: International Maritime Code for Dangerous Goods
  - DOT: US Department of Transportation
  - IATA: International Air Transport Association
  - ACGIH: American Conference of Governmental Industrial Hygienists
  - 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)
  - HMS: 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
  - TLV: Threshold Limit Value
  - PEL: Permissible Exposure Limit
  - REL: Recommended Exposure Limit
  - Flam. Liq. 2: Flammable liquids – Category 2
  - Eye Irrit. 2A: Serious eye damage/eye irritation – Category 2A
  - STOT SE 3: Specific target organ toxicity (single exposure) – Category 3
- **\* Data compared to the previous version altered.**

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