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Revision date 02/03/2023

Safety Data Sheet acc. to OSHA HCS

Printing date 02/03/2023

1 Identification

· Product identifier

Trade name: 9(S)-PAHSA

· Article number: 18023

· 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

2 Hazard(s) identification

· Classification of the substance or mixture



GHS02 Flame

Flammable Liquids 2 H225 Highly flammable liquid and vapor.



Eye Irritation 2A

H319 Causes serious eye irritation.

Specific Target Organ Toxicity - Single Exposure 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).

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Trade name: 9(S)-PAHSA

· Hazard pictograms



· Signal word Danger

Hazard-determining components of labeling:

Methyl acetate

· Hazard statements

H225 Highly flammable liquid and vapor.

H319 Causes serious eye irritation.

H336 May cause drowsiness or dizziness.

Precautionary statements

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

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.

P271 Use only outdoors or in a well-ventilated area.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

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.

P312 Call a poison center/doctor if you feel unwell.

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+P233 Store in a well-ventilated place. Keep container tightly closed.

P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

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

· Other hazards

- · Results of PBT and vPvB assessment
- · **PBT:** Not applicable.

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· **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 compor 	nents:	
CAS: 79-20-9	Methyl acetate	99.9%
RTECS: Al9100000		

· Other ingredients

2097130-87-3 9S-[(1-oxohexadecyl)oxy]-octadecanoic acid

0.1%

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

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:

CO2, 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 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

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.

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See Section 13 for disposal information.

· Protective Action Criteria for Chemicals

· PAC-1·

· PAC-1:	
79-20-9 Methyl acetate	250 ppm
· PAC-2:	
79-20-9 Methyl acetate	1,700 ppm
· 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
- · 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 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/m³, 200 ppm REL Short-term value: 760 mg/m³, 250 ppm Long-term value: 610 mg/m³, 200 ppm

TLV Short-term value: 250 ppm

Long-term value: 250 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 eves.

Avoid contact with the eyes and skin.

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Breathing equipment:

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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

9 Physical and chemical properties

- · Information on basic physical and chemical properties
- · General Information
- · Appearance:

Form: Liquid Color: Colorless · Odor: Pleasant · Structural Formula C34H66O4 · Molecular Weight 538.9 g/mol · 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: 57 °C (134.6 °F) · Flash point: -13 °C (8.6 °F) · Flammability (solid, gaseous): Highly flammable. · Ignition temperature: 455 °C (851 °F) · Decomposition temperature: Not determined.

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Auto igniting:	Product is not selfigniting.
Danger of explosion:	Product is not explosive. However, formation of explosive air vapor mixtures are possible.
Explosion limits:	
Lower:	3.1 Vol %
Upper:	16 Vol %
Vapor pressure at 20 °C (68 °F):	220 hPa (165 mm Hg)
Density at 20 °C (68 °F):	0.93 g/cm³ (7.76085 lbs/gal)
Bulk density:	1 kg/m³
Relative density	Not determined.
Vapor density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water at 20 °C (68 °F):	330 g/l
Partition coefficient (n-octanol/wat	er): Not determined.
Viscosity:	
Dynamic:	Not determined.
Kinematic:	Not determined.
SOLUBILITY	DMSO: 15 mg/ml; DMF: 20 mg/ml; Ethanol:PBS(pH 7.2) (
	1): 0.5 mg/ml; Ethanol: 20 mg/ml
Solvent content:	
Organic solvents:	99.9 %
VOC content:	0.00 %
	0.0 g/l / 0.00 lb/gal
Solids content:	0.0 %
Other information	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: acids; alkalis; nitrates; strong oxidizing agents
- · Hazardous decomposition products: carbon dioxide; carbon monoxide

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11 Toxicological information

- · Information on toxicological effects
- · Acute toxicity:

· LD/LC50 values that are relevant for classification:				
79-20-9 Methyl acetate				
Oral	LD50	>5,000 mg/kg (rat)		
		3,705 mg/kg (rabbit)		
Dermal	LD50	>5,000 mg/kg (rabbit)		
Inhalative	TCLO	15,000 mg/m³ (hmn)		
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.

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· Other adverse effects No further relevant information available.

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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.

UN-Number		
DOT, IMDG, IATA	UN1231	
UN proper shipping name		
DOT, IATA	Methyl acetate solution	
IMDG	METHYL ACETATE solution	
Transport hazard class(es)		
DOT		
FLAMMARIE LOUID		
3		
Class	3 Flammable liquids	
Label	3	
IMDG, IATA		
3		
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 co	ode): 33	
EMS Number:	F-E,S-D	
Stowage Category	В	

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· Transport/Additional information:	
· DOT	
· Quantity limitations	On passenger aircraft/rail: 5 L On cargo aircraft only: 60 L
· IMDG · Limited quantities (LQ) · Excepted quantities (EQ)	1L 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 m or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minim Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled a Dangerous Goods/Excepted Quantity.
· UN "Model Regulation":	UN 1231 METHYL ACETATE 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):

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.

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· TLV (Threshold Limit Value)

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

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 02/03/2023
- 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

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit REL: Recommended Exposure Limit

Flammable Liquids 2: Flammable liquids - Category 2

Eye Irritation 2A: Serious eye damage/eye irritation - Category 2A

Specific Target Organ Toxicity - Single Exposure 3: Specific target organ toxicity (single exposure) - Category 3