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1 Identification

- · Product identifier
- Trade name: <u>12(S)-HETE-d8</u>
- Article number: 334570
- **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		
H225 Highly flammable liquid and vapor.		
H302 Harmful if swallowed.		
H312 Harmful in contact with skin.		
H332 Harmful if inhaled.		
H319 Causes serious eye irritation.		
d labeled according to the Globally Harmonized System (GHS). (Contd. on page 2)		

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Safety Data Sheet acc. to OSHA HCS

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	= 1 E-08
· Hazard pictogran	(Contd. from page 1)
GHS02 GHS07	
· Signal word Dang	jer
· Hazard-determini	ing components of labeling:
Acetonitrile	
 Hazard statemen 	ts
H225	Highly flammable liquid and vapor.
H302+H312+H332	2 Harmful if swallowed, in contact with skin or if inhaled.
H319	Causes serious eye irritation.
• Precautionary sta	atements
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.
	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 (sc 	
A 1.1 1.	
	th = 2
Fire :	
Read	stivity = 0
HMIS-ratings (sc	ale 0 - 4)
HEALTH 2 Hea	lth = 2
FIRE 3 Fire	
REACTIVITY 0 Rea	activity = 0

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99.99%

0.01%

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- · 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: 75-05-8 Acetonitrile

RTECS: AL7700000

Other ingredients

84807-90-9 12(S)-HETE-d8

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

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:

CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

- Special hazards arising from the substance or mixture No further relevant information available.
- Advice for firefighters
- Protective equipment: Mouth respiratory protective device.

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	al precautions, protective equipment and emergency procedures	
	otective equipment. Keep unprotected persons away.	
	mental precautions:	
	th plenty of water. llow to enter sewers/ surface or ground water.	
	s and material for containment and cleaning up:	
Absorb v Dispose	with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust). contaminated material as waste according to item 13. adequate ventilation.	
	ce to other sections	
	tion 7 for information on safe handling.	
	tion 8 for information on personal protection equipment.	
See Sec	tion 13 for disposal information.	
Protecti	ve Action Criteria for Chemicals	
PAC-1:		
75-05-8	Acetonitrile 13 p	opn
PAC-2:		
75-05-8	Acetonitrile 50 p	ppn
PAC-3:		
75-05-8	Acetonitrile 150 p	opr

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:

75-05-8 Acetonitrile

PEL Long-term value: 70 mg/m³, 40 ppm

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REL Long-term value: 34 mg/m ³ , 2	
TLV Long-term value: 20 ppm Skin, A4	
· Additional information: The lists t	that were valid during the creation were used as basis.
 Exposure controls Personal protective equipment: General protective and hygienic Keep away from foodstuffs, bevera Immediately remove all soiled and a Wash hands before breaks and at Avoid contact with the eyes. Avoid contact with the eyes and ski Breathing equipment: In case of brief exposure or low p 	measures: ges and feed. contaminated clothing. the end of work.
The glove material has to be imper Due to missing tests no recomm preparation/ the chemical mixture. Selection of the glove material or degradation • Material of gloves The selection of the suitable glove quality and varies from manufact substances, the resistance of the g be checked prior to the application. • Penetration time of glove materia	
9 Physical and chemical prop	perties
 Information on basic physical an General Information Appearance: Form: Color: Odor: Structural Formula Molecular Weight 	Liquid Colorless Aromatic C20H24D8O3 328.5 g/mol
· Odor threshold:	Not determined.
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· Formulation	A solution in acetonitrile	
· pH-value:	Not determined.	
 Change in condition Melting point/Melting range: Boiling point/Boiling range: 	-46 °C (-50.8 °F) 81 °C (177.8 °F)	
· Flash point:	5 °C (41 °F)	
· Flammability (solid, gaseous):	Highly flammable.	
· Ignition temperature:	525 °C (977 °F)	
· Decomposition temperature:	Not determined.	
· Auto igniting:	Product is not selfigniting.	
[.] Danger of explosion:	Product is not explosive. However, formation of explosive ai vapor mixtures are possible.	
· Explosion limits: Lower: Upper:	4.4 Vol % 16 Vol %	
· Vapor pressure at 20 °C (68 °F):	97 hPa (72.8 mm Hg)	
 Density at 20 °C (68 °F): Relative density Vapor density Evaporation rate 	0.7822 g/cm³ (6.52746 lbs/gal) Not determined. Not determined. Not determined.	
 Solubility in / Miscibility with Water: 	Fully miscible.	
· Partition coefficient (n-octanol/water): Not determined.		
[·] Viscosity: Dynamic at 20 °C (68 °F): Kinematic: SOLUBILITY	0.39 mPas Not determined. 0.1 M Na2CO3: 2 mg/ml; DMF: Miscible; DMSO: Miscible Ethanol: Miscible; PBS pH 7.2: 0.8 mg/ml	
 Solvent content: 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: bases, oxidizing agents, reducing agents,

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· Hazardous decomposition products:

carbon dioxide, carbon monoxide, hydrogen cyanide, nitrogen oxides

11 Toxicological information

Information on toxicological effects

• Acute toxicity:

ATE (Acute Toxicity Estimate)		
Oral	LD50	2,460 mg/kg (rat)
Dermal	LD50	2,460 mg/kg (rat) 980 mg/kg (rabbit)
Inhalative	LC50/4 h	11 mg/l

75-05-8 Acetonitrile

Oral	TDLO	64 ml/kg (man)
	LD50	2,460 mg/kg (rat)
Dermal	LD50	980 mg/kg (rabbit)
Inhalative	LC50/4 h	7,551 mg/m³ (rat)
	LC50	7,551 mg/m³/8h (rat)
	TCLO	160 mg/m³/4h (hmn)
Irritation of eyes	Irritation	100 µl/24 hr (rabbit)
	Irritation	100 ìl/24 hr (rabbit)

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.

12 Ecological information

· Toxicity

- Aquatic toxicity: No further relevant information available.
- Persistence and degradability No further relevant information available.
- Behavior in environmental systems:
- \cdot Bioaccumulative potential No further relevant information available.
- Mobility in soil No further relevant information available.

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- · 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.

UN-Number DOT, IMDG, IATA	UN1648	
UN proper shipping name		
DOT, IATA	Acetonitrile solution	
IMDG	ACETONITRILE solution	
Transport hazard class(es)		
DOT		
Class	3 Elammable liquida	
Label	3 Flammable liquids 3	
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	

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 Hazard identification number (Kemler code): EMS Number: Stowage Category Stowage Code 	33 F-E,S-D B 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) 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 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	
· 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.	
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· 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 10/13/2022

· 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 Acute Toxicity - Oral 4: Acute toxicity - Category 4 Eye Irritation 2A: Serious eye damage/eye irritation - Category 2A

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