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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 5-(((13,13,14,14,15,15,16,16,16-d9)palmitoyl)hydroxy]-stearic acid

Product Number : 860410C

Brand : Avanti

REACH No. :

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

Uses advised against : For R&D use only. Not for pharmaceutical, household or other uses.

1.3

1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Acute toxicity, (Category 4) H302: Harmful if swallowed.

Acute toxicity, (Category 3) H331: Toxic if inhaled.

Skin irritation, (Category 2) H315: Causes skin irritation.

Eye irritation, (Category 2) H319: Causes serious eye irritation.

Carcinogenicity, (Category 2) H351: Suspected of causing cancer.

Reproductive toxicity, (Category 2) H361d: Suspected of damaging the unborn child.

Specific target organ toxicity -
single exposure, (Category 3),
Respiratory system

H336: May cause drowsiness or dizziness.

Specific target organ toxicity -
repeated exposure, (Category 1),
Liver, Kidney

H372: Causes damage to organs through
prolonged or repeated exposure if
swallowed.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H336	May cause drowsiness or dizziness.
H351	Suspected of causing cancer.
H361d	Suspected of damaging the unborn child.
H372	Causes damage to organs (Liver, Kidney) through prolonged or repeated exposure if swallowed.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P302 + P352	IF ON SKIN: Wash with plenty of water.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
Supplemental Hazard Statements	none
	For use in industrial installations only.

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word	Danger
Hazard Statements	
H331	Toxic if inhaled.
H351	Suspected of causing cancer.
H372	Causes damage to organs through prolonged or repeated exposure if swallowed.
H361d	Suspected of damaging the unborn child.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.

P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : 5-PAHSA-d9

Component		Classification	Concentration
Chloroform			
CAS-No.	67-66-3	Acute Tox. 4; Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2; Carc. 2; Repr. 2; STOT SE 3; STOT RE 1; H302, H331, H315, H319, H351, H361d, H336, H372 Concentration limits: 20 %: STOT SE 3, H336;	>= 90 - <= 100 %
EC-No.	200-663-8		
Index-No.	602-006-00-4		
Registration number	01-2119486657-20-XXXX		

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures**5.1 Extinguishing media****Suitable extinguishing media**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen chloride gas

Not combustible.

Ambient fire may liberate hazardous vapours.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage**7.1 Precautions for safe handling****Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability Recommended storage temperature
-20 °C

Storage class

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

required

Body Protection

protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type AX

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|-------------------|-----------|
| a) Physical state | liquid |
| b) Color | colorless |
| c) Odor | sweet |

d) Melting point/freezing point	Melting point: -63,5 °C at 1.013 hPa
e) Initial boiling point and boiling range	61,2 °C at 1.013 hPa
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	- DIN 51755 Part 1 does not flash Not applicable
i) Autoignition temperature	> 600 °C at 1.013 hPa - DIN 51794 Not applicable
j) Decomposition temperature	Distillable in an undecomposed state at normal pressure.
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	8,7 g/l at 23 °C - OECD Test Guideline 105
n) Partition coefficient: n-octanol/water	log Pow: 1,97 at 25 °C - (ECHA), Bioaccumulation is not expected.
o) Vapor pressure	210 hPa at 20 °C
p) Density	1,49 g/cm ³
Relative density	No data available
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

Solubility in other solvents	organic solvent at 20 °C - miscible
Surface tension	27,1 mN/m at 20,0 °C
Relative vapor density	4,12 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong oxidizing agents, Strong bases, Magnesium, Sodium/sodium oxides, Lithium, various plastics

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 908 mg/kg
(Calculation method)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute toxicity estimate Inhalation - 4 h - 3,1 mg/l - vapor (Calculation method)

Symptoms: Possible symptoms:, mucosal irritations

Dermal: No data available

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

Evidence of a carcinogenic effect.

Reproductive toxicity

Evidence of harm to the unborn child.

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Mixture causes damage to organs through prolonged or repeated exposure.

- Liver, Kidney

Aspiration hazard

No data available

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components

Chloroform

Acute toxicity

LD50 Oral - Rat - male - 908 mg/kg

(OECD Test Guideline 401)

Acute toxicity estimate Oral - 908 mg/kg

(ATE value derived from LD50/LC50 value)

LC50 Inhalation - Rat - 6 h - 9,17 mg/l - vapor

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 3,1 mg/l - vapor

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: (ECHA)

Remarks: Drying-out effect resulting in rough and chapped skin.

Skin - Rabbit

Result: slight irritation

Remarks: (IUCLID)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

Remarks: (ECHA)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(Regulation (EC) No. 440/2008, Annex, B.6)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Result: negative

Remarks: (ECHA)

Test Type: unscheduled DNA synthesis assay

Test system: Liver

Result: negative

Remarks: (ECHA)

Method: OECD Test Guideline 474

Species: Rat - male and female - Red blood cells (erythrocytes)

Result: negative

Method: OECD Test Guideline 486

Species: Rat - male - Liver cells

Result: negative

Species: Mouse - female

Result: negative

Remarks: (ECHA)

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Oral - Causes damage to organs through prolonged or repeated exposure.

- Liver, Kidney

Aspiration hazard

No data available

SECTION 12: Ecological information**12.1 Toxicity****Mixture**

No data available

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties**Product:**

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

No data available

Components**Chloroform**

Toxicity to daphnia
and other aquatic
invertebrates

static test EC50 - Crassostrea gigas - 152,5 mg/l - 48 h
Remarks: (ECHA)

Toxicity to algae

static test ErC50 - Chlamydomonas reinhardtii (green algae) -
13,3 mg/l - 72 h
Remarks: (ECHA)

Toxicity to daphnia
and other aquatic
invertebrates(Chronic

semi-static test NOEC - Daphnia magna (Water flea) - 6,3 mg/l
- 21 d
Remarks: (ECHA)

toxicity)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1888

IMDG: 1888

IATA: 1888

14.2 UN proper shipping name

ADR/RID: CHLOROFORM, SOLUTION

IMDG: CHLOROFORM, SOLUTION

IATA: Chloroform, SOLUTION

14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA: 6.1

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (E)

Further information : No data available

14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Authorisations and/or restrictions on use

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII) : Chloroform

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

H2 ACUTE TOXIC

H2 ACUTE TOXIC

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H336	May cause drowsiness or dizziness.
H351	Suspected of causing cancer.
H361d	Suspected of damaging the unborn child.
H372	Causes damage to organs through prolonged or repeated exposure if swallowed.

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

Classification of the mixture

Acute Tox.4	H302
Acute Tox.3	H331
Skin Irrit.2	H315
Eye Irrit.2	H319
Carc.2	H351
Repr.2	H361d
STOT SE3	H336
STOT RE1	H372

Classification procedure:

Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method

CHEMIKART