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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : (E)-4R-hydroxynonenal-dimethylacetal (Each vial contains 6.8mg which yields ~5.2mg 4-HNE after deprotection)

Product Number : 870608H
Brand : Avanti
REACH No. : This product is a mixture. REACH Registration Number see section 3.

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**

Flammable liquids, (Category 2) H225: Highly flammable liquid and vapor.

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

Reproductive toxicity, (Category 2) H361f: Suspected of damaging fertility.

Specific target organ toxicity - single exposure, (Category 3), H336: May cause drowsiness or dizziness.

Central nervous system

Specific target organ toxicity - repeated exposure, (Category 1), Nervous system

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

Aspiration hazard, (Category 1)

H304: May be fatal if swallowed and enters airways.

Long-term (chronic) aquatic hazard, (Category 2)

H411: Toxic to aquatic life with long lasting effects.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H361f	Suspected of damaging fertility.
H372	Causes damage to organs (Nervous system) through prolonged or repeated exposure if inhaled.
H411	Toxic to aquatic life with long lasting effects.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P273	Avoid release to the environment.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P331	Do NOT induce vomiting.
Supplemental Hazard Statements	none

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word	Danger
Hazard Statements	
H372	Causes damage to organs through prolonged or repeated exposure if inhaled.
H304	May be fatal if swallowed and enters airways.
H361f	Suspected of damaging fertility.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P331	Do NOT induce vomiting.

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 : 4-HNE-dimethylacetal

Molecular weight : 86,18 g/mol

Component		Classification	Concentration
n-Hexane			
CAS-No.	110-54-3	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 1; Asp. Tox. 1; Aquatic Chronic 2; H225, H315, H361f, H336, H372, H304, H411 Concentration limits: >= 5 %: STOT RE 2, H373; >= 20 %: STOT SE 3, H336;	>= 90 - <= 100 %
EC-No.	203-777-6		
Index-No.	601-037-00-0		
Registration number	01-2119480412-44-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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

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: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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

Foam Carbon dioxide (CO₂) Dry powder

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

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

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

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition.

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. Risk of explosion.

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.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. 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): 3: Flammable liquids

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

Flame retardant antistatic 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 ABEK

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. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|-------------------|-------------------|
| a) Physical state | liquid |
| b) Color | colorless |
| c) Odor | No data available |

- | | |
|---|--|
| d) Melting point/freezing point | -95,0 °C |
| e) Initial boiling point and boiling range | 68,0 - 70,0 °C |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 7,7 %(V)
Lower explosion limit: 1,2 %(V) |
| h) Flash point | -26,0 °C - closed cup |
| i) Autoignition temperature | 234,0 °C |
| j) Decomposition temperature | No data available |
| k) pH | 7,0 |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: No data available |
| m) Water solubility | insoluble |
| n) Partition coefficient: n-octanol/water | log Pow: 3,90 - 4,11 |
| o) Vapor pressure | 341,3 hPa at 37,7 °C
176,0 hPa at 20,0 °C |
| p) Density | 0,65 g/cm ³ |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| | |
| s) Explosive properties | Not classified as explosive. |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

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

Warming.

10.5 Incompatible materials

Strong oxidizing agents

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

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

Evidence to impair fertility.

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.

- Nervous system

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

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

n-Hexane

Acute toxicity

LD50 Oral - Rat - male and female - 16.000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - 172 mg/l - vapor

Remarks: (RTECS)

LD50 Dermal - Rabbit - male - > 2.000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 24 h

(OECD Test Guideline 404)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h

(OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 478

Species: Mouse - male

Result: negative

Method: OECD Test Guideline 475

Species: Rat - male and female - Bone marrow

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

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

- Nervous system

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

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

n-Hexane

Toxicity to fish

LC50 - Pimephales promelas (fathead minnow) - 2,5 mg/l - 96 h
Remarks: (ECOTOX Database)

Toxicity to daphnia
and other aquatic
invertebrates

EC50 - Daphnia magna (Water flea) - 2,1 mg/l - 48 h
Remarks: (Lit.)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1208

IMDG: 1208

IATA: 1208

14.2 UN proper shipping name

ADR/RID: HEXANES, SOLUTION

IMDG: HEXANES, SOLUTION
IATA: Hexanes, SOLUTION

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

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

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.	P5c	FLAMMABLE LIQUIDS
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E2 ENVIRONMENTAL HAZARDS

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

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H361f	Suspected of damaging fertility.
H372	Causes damage to organs through prolonged or repeated exposure if inhaled.
H373	May cause damage to organs through prolonged or repeated exposure.

Relevant changes since previous version

2. Hazards identification

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