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

Product name : omega(7-nitro-2-1,3-benzoxadiazol-4-yl)(2S,3R,4E)-2-aminooctadec-4-ene-1,3-diol

Product Number : 810205X

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.

Acute toxicity, (Category 4) H312: Harmful in contact with skin.

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 1)	H370: Causes damage to organs.
Specific target organ toxicity - single exposure, (Category 3), Central nervous system	H336: May cause drowsiness or dizziness.
Specific target organ toxicity - repeated exposure, (Category 1)	H372: Causes damage to organs through prolonged or repeated exposure.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H302 + H312	Harmful if swallowed or in contact with skin.
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.
H370	Causes damage to organs.
H372	Causes damage to organs through prolonged or repeated exposure.
Precautionary Statements	
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
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 + P311	IF exposed or concerned: Call a POISON CENTER/ doctor.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
Supplemental Hazard Statements	none
	For use in industrial installations only.

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 : NBD Sphingosine

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;	>= 70 - < 90 %
EC-No.	200-663-8		
Index-No.	602-006-00-4		
Registration number	01-2119486657-20-XXXX		
Methanol			
CAS-No.	67-56-1	Flam. Liq. 2; Acute Tox. 3; STOT SE 1; H225, H301, H331, H311, H370 Concentration limits: >= 10 %: STOT SE 1, H370; 3 - < 10 %: STOT SE 2, H371;	>= 20 - < 30 %
EC-No.	200-659-6		
Index-No.	603-001-00-X		
Registration number	01-2119433307-44-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

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. Call a physician immediately.

In case of eye contact

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

If swallowed

After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour). 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

Water 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

Hydrogen chloride gas

Mixture with combustible ingredients.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

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. 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. 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 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. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- a) Physical state liquid

b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	51,95 °C
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	> 51,95 °C
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient: n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	1,35 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

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .
Contains the following stabilizer(s):
ethanol (0,5 %)

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heating.

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

Acute toxicity estimate Oral - 347,37 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

Acute toxicity estimate Dermal - 1.501 mg/kg

(Calculation method)

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 causes damage to organs.

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Mixture causes damage to organs through prolonged or repeated exposure.

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

Methanol**Acute toxicity**

Acute toxicity estimate Oral - 100,1 mg/kg

(Expert judgment)

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

Symptoms: Nausea, Vomiting

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

(Expert judgment)

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

Symptoms: Irritation symptoms in the respiratory tract.

Acute toxicity estimate Dermal - 300,1 mg/kg

(Expert judgment)

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

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks: (ECHA)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Remarks: (ECHA)

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Based on available data the classification criteria are not met.

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Bone marrow

Result: negative

Carcinogenicity

Did not show carcinogenic effects in animal experiments.

Reproductive toxicity

Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

Causes damage to organs. - Eyes, Central nervous system

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

Acute oral toxicity - Nausea, Vomiting

Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure

No data available

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)

Methanol

Toxicity to fish	flow-through test LC50 - <i>Lepomis macrochirus</i> (Bluegill) - 15.400,0 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - 18.260 mg/l - 96 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - ca. 22.000,0 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test IC50 - activated sludge - > 1.000 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	NOEC - <i>Oryzias latipes</i> (Orange-red killifish) - 7.900 mg/l - 200 h Remarks: (External MSDS)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1992

IMDG: 1992

IATA: 1992

14.2 UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, TOXIC, N.O.S. (Chloroform, Methanol)

IMDG: FLAMMABLE LIQUID, TOXIC, N.O.S. (Chloroform, Methanol)

IATA: Flammable liquid, toxic, n.o.s. (Chloroform, Methanol)

14.3 Transport hazard class(es)

ADR/RID: 3 (6.1)

IMDG: 3 (6.1)

IATA: 3 (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 : (D/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
Methanol

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

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Methanol

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.
H301	Toxic if swallowed.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
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.
H370	Causes damage to organs.
H371	May cause damage to organs.
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
Acute Tox.4	H312
Skin Irrit.2	H315
Eye Irrit.2	H319
Carc.2	H351
Repr.2	H361d
STOT SE1	H370
STOT SE3	H336
STOT RE1	H372

Classification procedure:

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