

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.6

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1 Product identifiers

Product name : trans-11-Vaccenic Methyl Ester, 1 x 1 mL, 10 mg/mL, Heptane

Product Number : CRM46905

Brand : Supelco

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

CHEMIKART

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.

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

Aspiration hazard, (Category 1)	H304: May be fatal if swallowed and enters airways.
Short-term (acute) aquatic hazard, (Category 1)	H400: Very toxic to aquatic life.
Long-term (chronic) aquatic hazard, (Category 1)	H410: Very 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.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary Statements	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
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	
H304	May be fatal if swallowed and enters airways.
Precautionary Statements	
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

Molecular weight : 100,21 g/mol

Component		Classification	Concentration
n-heptane			
CAS-No.	142-82-5	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 Concentration limits: 20 %: STOT SE 3, H336; M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	>= 90 - <= 100 %
EC-No.	205-563-8		
Index-No.	601-008-00-2		
Registration number	01-2119457603-38-XXXX		
trans-Vaccenic acid methyl ester			
CAS-No.	6198-58-9	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
EC-No.	228-251-3		
	*		

*A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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.

In case of eye contact

After eye contact: rinse out with plenty of water. 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.

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 | No data available |
| c) Odor | No data available |
| d) Melting point/freezing point | -90,99 °C |
| e) Initial boiling point and boiling range | 98,0 - 99,0 °C |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 7 %(V)
Lower explosion limit: 1,1 %(V) |
| h) Flash point | -3,99 °C - closed cup |
| i) Autoignition temperature | 223,0 °C |
| 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 | insoluble |
| n) Partition coefficient: n-octanol/water | log Pow: > 3,000 |
| o) Vapor pressure | 110,7 hPa at 37,7 °C
53,3 hPa at 20,0 °C |

- | | |
|-----------------------------|------------------------------|
| p) Density | 0,68 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

No data available

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

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.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components**n-heptane****Acute toxicity**

LD50 Oral - Rat - male and female - > 5.000 mg/kg
(OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: isooctane
LC50 Inhalation - Rat - male and female - 4 h - > 29,29 mg/l - vapor
(OECD Test Guideline 403)

LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg
(OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: isooctane

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h
(OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: isooctane

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: isooctane

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Remarks: **Germ cell mutagenicity**

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: rat hepatocytes

Result: negative

Carcinogenicity

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

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

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways. Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

trans-Vaccenic acid methyl ester**Acute toxicity**

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

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**n-heptane**

No data available

trans-Vaccenic acid methyl ester

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1206

IMDG: 1206

IATA: 1206

14.2 UN proper shipping name

ADR/RID: HEPTANES, SOLUTION

IMDG: HEPTANES, SOLUTION

IATA: Heptanes, 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.

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.

E1 ENVIRONMENTAL HAZARDS

P5c FLAMMABLE LIQUIDS

Other regulations

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.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

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

Flam. Liq.2	H225
Skin Irrit.2	H315
STOT SE3	H336
Asp. Tox.1	H304
Aquatic Acute1	H400
Aquatic Chronic1	H410

Classification procedure:

Based on product data or assessment
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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