

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 8.5
Revision Date 24.07.2023
Print Date 24.07.2023**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : A-PHELLANDRENE FOR SYNTHESIS

Product Number : 8.14893

Catalogue No. : 814893

Brand : Millipore

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 99-83-2

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

Identified uses : Chemical for synthesis

1.3 Details of the supplier of the safety data sheet

Company : Merck Life Science UK Limited
New Road
The Old Brickyard
GILLINGHAM
Dorset
SP8 4XT
UNITED KINGDOM

Telephone : +44 (0)1747 833-000

Fax : +44 (0)1747 833-313

E-mail address : TechnicalService@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : +44 (0)870 8200418 (CHEMTREC)

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture**

Classification according to Regulation (EC) No 1272/2008 as amended by GB-CLP Regulation, UK SI 2019/720, and UK SI 2020/1567

Flammable liquids (Category 3), H226
Skin irritation (Category 2), H315
Skin sensitization (Category 1), H317
Reproductive toxicity (Category 2), H361

Aspiration hazard (Category 1), H304
Long-term (chronic) aquatic hazard (Category 2), H411

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008 as amended by GB-CLP Regulation, UK SI 2019/720, and UK SI 2020/1567

Pictogram



Signal Word Danger

Hazard statement(s)

H226 Flammable liquid and vapor.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H361 Suspected of damaging fertility or the unborn child.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
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 statement(s)

H317 May cause an allergic skin reaction.
H361 Suspected of damaging fertility or the unborn child.
H304 May be fatal if swallowed and enters airways.

Precautionary statement(s)

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
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

3.1 Substances

Formula : C₁₀H₁₆
Molecular weight : 136.23 g/mol
CAS-No. : 99-83-2
EC-No. : 202-792-5

Component	Classification	Concentration
p-mentha-1,5-diene		
CAS-No. 99-83-2 EC-No. 202-792-5	Flam. Liq. 3; Asp. Tox. 1; H226, H304	>= 70 - < 90 %
p-Cymene		
CAS-No. 99-87-6 EC-No. 202-796-7 Index-No. 601-094-00-1	Flam. Liq. 3; Acute Tox. 3; Repr. 2; Asp. Tox. 1; Aquatic Chronic 2; H226, H331, H361f, H304, H411 Acute inhalation toxicity(vapor): 3 mg/l	>= 10 - < 20 %
(1S)-(-)-α-pinene		
CAS-No. 7785-26-4 EC-No. 232-077-3	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 2; H226, H302, H315, H304, H400, H411 M-Factor - Aquatic Acute: 1	>= 2.5 - < 10 %
p-mentha-1,4(8)-diene		
CAS-No. 586-62-9 EC-No. 209-578-0	Skin Sens. 1; Asp. Tox. 1; Aquatic Acute 1; Aquatic	>= 2.5 - < 10 %

		Chronic 3; H317, H304, H400, H412 M-Factor - Aquatic Acute: 1	
7-methyl-3-methyleneocta-1,6-diene			
CAS-No.	123-35-3	Flam. Liq. 3; Skin Irrit. 2; Eye Irrit. 2; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H226, H315, H319, H304, H400, H410	≥ 2.5 - < 10 %
EC-No.	204-622-5		
p-mentha-1,4-diene			
CAS-No.	99-85-4	Flam. Liq. 3; Repr. 2; Aquatic Chronic 2; H226, H361, H411	≥ 3 - < 10 %
EC-No.	202-794-6		

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.

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. 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 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.

Recommended storage temperature see product label.

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**

Contains no substances with occupational exposure limit values.

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

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 | No data available |
| e) Initial boiling point and boiling range | 175 °C at 1,013 hPa |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower | No data available |

	flammability or explosive limits	
h)	Flash point	47 °C
i)	Autoignition temperature	No data available
j)	Decomposition temperature	No data available
k)	pH	at 20 °C neutral
l)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m)	Water solubility	No data available
n)	Partition coefficient: n-octanol/water	log Pow: 4.62 - Potential bioaccumulation, (Lit.)
o)	Vapor pressure	No data available
p)	Density	0.84 g/cm ³ at 20 °C
	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

Sensitivity to light

Sensitive to air.

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

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Bases

Acids

10.4 Conditions to avoid

Exposure to light.

Heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - > 2,000 mg/kg

(Calculation method)

LD50 Oral - Rat - 5,700 mg/kg (p-mentha-1,5-diene)

Symptoms: Nausea, Vomiting

Remarks: (External MSDS)

Acute toxicity estimate Inhalation - 4 h - > 20 mg/l - vapor(Calculation method)

Dermal: No data available

Skin corrosion/irritation

Skin - Human (p-mentha-1,5-diene)

Result: Severe irritations

Remarks: (RTECS)

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

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis. (p-mentha-1,5-diene)

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.

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (p-mentha-1,5-diene)

Possible effects:

(p-mentha-1,5-diene)

Irritations

Allergic reactions

Nausea

Vomiting

Aspiration may cause pulmonary edema and pneumonitis.

(p-mentha-1,5-diene)

Other dangerous properties can not be excluded.

(p-mentha-1,5-diene)

Handle in accordance with good industrial hygiene and safety practice.

(p-mentha-1,5-diene)

SECTION 12: Ecological information

12.1 Toxicity

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

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations**13.1 Waste treatment methods****Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. Notice Directive on waste 2008/98/EC.

SECTION 14: Transport information**14.1 UN number**

ADR/RID: 1993

IMDG: 1993

IATA: 1993

14.2 UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, N.O.S. (p-mentha-1,5-diene)

IMDG: FLAMMABLE LIQUID, N.O.S. (p-mentha-1,5-diene)

IATA: Flammable liquid, n.o.s. (p-mentha-1,5-diene)

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

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.

P5c

FLAMMABLE LIQUIDS

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 referred to under sections 2 and 3.

H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H315	Flammable liquid and vapor.
H317	May be fatal if swallowed and enters airways.
H319	Causes skin irritation.
H331	May cause an allergic skin reaction.
H361	Causes serious eye irritation.
H361f	Toxic if inhaled.
H400	Suspected of damaging fertility or the unborn child.
H410	Suspected of damaging fertility.
H411	Flammable liquid and vapor.
H412	May be fatal if swallowed and enters airways.

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

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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Millipore- 8.14893

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