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Acetic acid linalyl ester ROTICHROM®GC for gas chromatography

article number: 5199 date of compilation: 2016-02-25 Version: GHS 5.0 en Revision: 2024-03-02

Replaces version of: 2021-08-26

Version: (GHS 4)

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

Product identifier 1.1

Identification of the substance Acetic acid linalyl ester ROTICHROM®GC for

gas chromatography

Article number 5199

CAS number 115-95-7

Alternative name(s) Linalylacetate

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

Relevant identified uses: Laboratory chemical

Laboratory and analytical use

Uses advised against: Do not use for private purposes (household).

Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG Schoemperlenstr. 3-5 D-76185 Karlsruhe Germany

Telephone:+49 (0) 721 - 56 06 0 **Telefax:** +49 (0) 721 - 56 06 149 e-mail: sicherheit@carlroth.de Website: www.carlroth.de

sheet:

sicherheit@carlroth.de e-mail (competent person):

1.4 **Emergency telephone number**

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 West- mead, NSW	131126	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	4	Flam. Liq. 4	H227
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315
3.3	Serious eye damage/eye irritation	2A	Eye Irrit. 2A	H319
3.45	Skin sensitisation	1	Skin Sens. 1	H317

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For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling

Signal word Warning

Pictograms

GHS07



Hazard statements

H227	Combustible liquid
H315	Causes skin irritation
H317	May cause an allergic skin reaction

H319 Causes serious eye irritation

Precautionary statements

Precautionary statements - prevention

P210	Keep away from heat/sparks/open flames/hot surfaces No smoking
P261	Avoid breathing dust/fume/gas/mist/vapours/spray

P280 Wear protective gloves

Precautionary statements - response

P302+P352	IF ON SKIN: Wash with plenty of soap and water
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact
	lenses, if present and easy to do. Continue rinsing
P333+P313	If skin irritation or rash occurs: Get medical advice/attention
P337+P313	If eye irritation persists: Get medical advice/attention
P370+P378	In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction

Precautionary statements - disposal

P501 Dispose of contents/container to industrial combustion plant

2.3 Other hazards

This material is combustible, but will not ignite readily.

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Acetic acid linalyl ester

Molecular formula $C_{12}H_{20}O_2$ Molar mass $196.3 \, ^{9}/_{mol}$ CAS No 115-95-7

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. After contact with skin, wash immediately with plenty of water. In case of skin irritation, consult a physician.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Irritation, Allergic reactions

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings! water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

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5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours may form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Do not breathe vapour/spray. Avoid contact with skin and eyes. Avoidance of ignition sources. Provide adequate ventilation.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

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Take precautionary measures against static discharge.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed. Keep in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 2 - 8 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

Human health values

Relevant DNELs and other threshold levels						
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time		
DNEL	2.75 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects		
DNEL	2.5 mg/kg bw/ day	human, dermal	worker (industry)	chronic - systemic effects		
DNEL	236.2 μg/cm²	human, dermal	worker (industry)	chronic - local effects		
DNEL	236.2 μg/cm²	human, dermal	worker (industry)	acute - local effects		

Environmental values

Relevant	Relevant PNECs and other threshold levels						
End- point	Threshold level	Organism	Environmental compartment	Exposure time			
PNEC	0.011 ^{mg} / _l	aquatic organisms	freshwater	short-term (single instance)			
PNEC	0.001 ^{mg} / _l	aquatic organisms	marine water	short-term (single instance)			
PNEC	1 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)			

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Relevant PNECs and other threshold levels

End- point	Threshold level	Organism	Environmental com- partment	Exposure time
PNEC	0.609 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.061 ^{mg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0.115 ^{mg} / _{kg}	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection





Use safety goggle with side protection.

Skin protection





hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

type of material

NBR (Nitrile rubber)

material thickness

0.4 mm

breakthrough times of the glove material

>480 minutes (permeation: level 6)

other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection





Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

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Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state liquid

Colour colourless
Odour mild sweet

Melting point/freezing point <-100 °C (ECHA)

Boiling point or initial boiling point and boiling 220 °C at 1,013 hPa (ECHA)

range

Flammability flammable liquid in accordance with GHS criteria

Lower and upper explosion limit not determined

Flash point 85 °C at 1,013 hPa (ECHA)

Auto-ignition temperature 270 °C at 1,012 mbar (ECHA)

Decomposition temperature not relevant

pH (value) not determined Kinematic viscosity 2.77 $^{\rm mm^2}/_{\rm s}$ at 20 $^{\circ}{\rm C}$

Dynamic viscosity 2.5 mPa s at 20 °C

Solubility(ies)

Water solubility 0.03 ^g/_l at 20 °C

Partition coefficient

Partition coefficient n-octanol/water (log value): 3.9 (25 °C) (ECHA)

Soil organic carbon/water (log KOC) 2.71 (ECHA)

Vapour pressure <1 hPa at 20 °C

Density and/or relative density

Density $0.902 \, {}^{9}/_{cm^3}$ at 20 ${}^{\circ}\text{C}$

Relative vapour density Information on this property is not available.

Particle characteristics not relevant (liquid)

Other safety parameters

Oxidising properties none

9.2 Other information

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Information with regard to physical hazard

classes:

Other safety characteristics:

There is no additional information.

There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Risk of ignition.

If heated

Risk of ignition. Vapours may form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Keep away from heat.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

Acute toxicity

Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	>9,000 ^{mg} / _{kg}	rat		ECHA
dermal	LD50	>5,000 ^{mg} / _{kg}	rabbit		ECHA

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

May cause an allergic skin reaction.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

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Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

If swallowed

Data are not available.

• If in eyes

Causes serious eye irritation

If inhaled

Data are not available.

• If on skin

causes skin irritation, May produce an allergic reaction, pruritis, localised redness

Other information

none

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
ErC50	62 ^{mg} / _l	algae	ECHA	72 h
LC50	11 ^{mg} / _l	fish	ECHA	96 h
EC50	59 ^{mg} / _I	aquatic invertebrates	ECHA	48 h

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
LC50	11.14 ^{mg} / _l	fish	ECHA	20 h

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12.2 Persistence and degradability

Theoretical Oxygen Demand: 2.608 ^{mg}/_{mg} Theoretical Carbon Dioxide: 2.69 ^{mg}/_{mg}

Biodegradation

The substance is readily biodegradable.

Process of degradability

Process	Degradation rate	Time
oxygen depletion	≥0 - ≤10 %	1 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3.9 (25 °C) (ECHA)
BCF	174 (ECHA)

12.4 Mobility in soil

Henry's law constant	176 ^{Pa m³} / _{mol} at 25 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	2.71 (ECHA)

12.5 Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0.1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

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SECTION 14: Transport information

14.1 UN number not subject to transport regulations

14.2 UN proper shipping name not assigned
 14.3 Transport hazard class(es) not assigned
 14.4 Packing group not assigned

14.5 Environmental hazards non-environmentally hazardous acc. to the dan-

gerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Transport informationNational regulationsAdditional information(UN RTDG)

Not subject to transport regulations. UN RTDG

International Maritime Dangerous Goods Code (IMDG) - Additional information

Not subject to IMDG.

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Not subject to ICAO-IATA.

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed

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Country	Inventory	Status
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC CICR CSCL-ENCS DSL ECSI IECSC Australian Inventory of Industrial Chemicals Chemical Inventory and Control Regulation List of Existing and New Chemical Substances (CSCL-ENCS)

CSCL-ENCS
DSL
Domestic Substances List (DSL)
ECSI
ECSI
ECS EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC
Inventory of Existing Chemical Substances Produced or Imported in China
INSQ
National Inventory of Chemical Substances
KECI
Korea Existing Chemicals Inventory
NCI
National Chemical Inventory
NZIOC
New Zealand Inventory of Chemicals
PICCS
Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.
REACH registered substances
TSI
Taiwan Chemical Substance Inventory
Toxic Substance Control Act

TCSI TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances

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Abbr.	Descriptions of used abbreviations
ErC50	≡ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H227	Combustible liquid.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.

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