

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



Acetoxyvalerenic acid ROTICHROM® HPLC

article number: **4446**
Version: **4.0 en**
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Version: (3)

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

1.1 Product identifier

Identification of the substance	Acetoxyvalerenic acid ROTICHROM® HPLC
Article number	4446
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
EC number	617-228-7
CAS number	81397-67-3

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

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

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

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Centre Beaumont Hospital	Beaumont Road	Dublin 9	+353 1 809 2166	https://www.poisons.ie/

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
4.1A	Hazardous to the aquatic environment - acute hazard	1	Aquatic Acute 1	H400
4.1C	Hazardous to the aquatic environment - chronic hazard	1	Aquatic Chronic 1	H410

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For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word

Warning

Pictograms

GHS09



Hazard statements

H410 Very toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P273 Avoid release to the environment

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Warning**

Symbol(s)



2.3 Other hazards

Special danger of slipping by leaking/spilling product.

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 $\geq 0,1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Acetoxyvalerenic acid
Molecular formula	$C_{17}H_{24}O_4$
Molar mass	292,4 g/mol
CAS No	81397-67-3
EC No	617-228-7

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SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

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

5.2 Special hazards arising from the substance or mixture

Combustible.

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. Do not allow firefighting water to enter drains or water courses. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

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SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

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.

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

No special measures are necessary.

Measures to protect the environment

Avoid release to the environment.

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 in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Specific designs for storage rooms or vessels

Recommended storage temperature: -20 °C

7.3 Specific end use(s)

No information available.

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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.

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

>0,11 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. Usually no personal respirative protection necessary.

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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
Form	viscous
Colour	colourless
Odour	odourless
Melting point/freezing point	not determined
Boiling point or initial boiling point and boiling range	not determined
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	not determined
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined
<u>Solubility(ies)</u>	
Water solubility	(practically insoluble)
Solubility in alcohol	soluble
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	this information is not available
Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	~1 g/cm ³ at 20 °C
Relative vapour density	Information on this property is not available.
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
Oxidising properties	none

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9.2 Other information

Information with regard to physical hazard classes:

hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics:

There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

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

UV-radiation/sunlight. Direct light irradiation. 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 hazard classes as defined in Regulation (EC) No 1272/2008

Classification according to GHS (1272/2008/EC, CLP)

Acute toxicity

Shall not be classified as acutely toxic.

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

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).

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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

Data are not available.

• If inhaled

Data are not available.

• If on skin

Data are not available.

• Other information

Health effects are not known.

11.2 Endocrine disrupting properties

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

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Very toxic to aquatic life with long lasting effects.

12.2 Persistence and degradability

Theoretical Oxygen Demand: $2,298 \text{ mg/mg}$
Theoretical Carbon Dioxide: $2,559 \text{ mg/mg}$

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

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.

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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. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

Properties of waste which render it hazardous

HP 14 ecotoxic

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.

SECTION 14: Transport information

14.1 UN number or ID number

ADRRID	UN 3082
IMDG-Code	UN 3082
ICAO-TI	UN 3082

14.2 UN proper shipping name

ADRRID	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
IMDG-Code	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
ICAO-TI	Environmentally hazardous substance, liquid, n.o.s.
Technical name	Acetoxyvalerenic acid

14.3 Transport hazard class(es)

ADRRID	9
IMDG-Code	9
ICAO-TI	9

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14.4 Packing group

ADRRID	III
IMDG-Code	III
ICAO-TI	III

14.5 Environmental hazards hazardous to the aquatic environment

14.6 Special precautions for user



Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime 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

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR) Additional information

Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
Particulars in the transport document	UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (Acetoxyvalerenic acid), 9, III, (-)
Classification code	M6
Danger label(s)	9, "Fish and tree"
 	
Environmental hazards	yes (hazardous to the aquatic environment)
Special provisions (SP)	274, 335, 375, 601
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
Transport category (TC)	3
Tunnel restriction code (TRC)	-
Hazard identification No	90

Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) Additional information

Classification code	M6
Danger label(s)	9, "Fish and tree"
 	
Environmental hazards	Yes Hazardous to water
Special provisions (SP)	274, 335, 375, 601
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L





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Transport category (TC)	3
Hazard identification No	90
International Maritime Dangerous Goods Code (IMDG) - Additional information	
Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.
Particulars in the shipper's declaration	UN3082, ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S., (Acetoxyvalerenic acid), 9, III
Marine pollutant	yes (hazardous to the aquatic environment), (Acetoxyvalerenic acid)
Danger label(s)	9, "Fish and tree"
 	
Special provisions (SP)	274, 335, 969
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
EmS	F-A, S-F
Stowage category	A
International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information	
Proper shipping name	Environmentally hazardous substance, liquid, n.o.s.
Particulars in the shipper's declaration	UN3082, Environmentally hazardous substance, liquid, n.o.s., (Acetoxyvalerenic acid), 9, III
Environmental hazards	yes (hazardous to the aquatic environment)
Danger label(s)	9, "Fish and tree"
 	
Special provisions (SP)	A97, A158, A197, A215
Excepted quantities (EQ)	E1
Limited quantities (LQ)	30 kg

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

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Dangerous substances with restrictions (REACH, Annex XVII)				
Name of substance	Name acc. to inventory	CAS No	Restriction	No
Acetoxyvalerenic acid	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		R3	3

Legend

- R3
1. Shall not be used in:
 - ornamental articles intended to produce light or colour effects by means of different phases, for example in ornamental lamps and ashtrays,
 - tricks and jokes,
 - games for one or more participants, or any article intended to be used as such, even with ornamental aspects,
 2. Articles not complying with paragraph 1 shall not be placed on the market.
 3. Shall not be placed on the market if they contain a colouring agent, unless required for fiscal reasons, or perfume, or both, if they:
 - can be used as fuel in decorative oil lamps for supply to the general public, and
 - present an aspiration hazard and are labelled with H304.
 4. Decorative oil lamps for supply to the general public shall not be placed on the market unless they conform to the European Standard on Decorative oil lamps (EN 14059) adopted by the European Committee for Standardisation (CEN).
 5. Without prejudice to the implementation of other Union provisions relating to the classification, labelling and packaging of substances and mixtures, suppliers shall ensure, before the placing on the market, that the following requirements are met:
 - (a) lamp oils, labelled with H304, intended for supply to the general public are visibly, legibly and indelibly marked as follows: "Keep lamps filled with this liquid out of the reach of children"; and, by 1 December 2010, "Just a sip of lamp oil – or even sucking the wick of lamps – may lead to life-threatening lung damage";
 - (b) grill lighter fluids, labelled with H304, intended for supply to the general public are legibly and indelibly marked by 1 December 2010 as follows: "Just a sip of grill lighter fluid may lead to life threatening lung damage";
 - (c) lamps oils and grill lighters, labelled with H304, intended for supply to the general public are packaged in black opaque containers not exceeding 1 litre by 1 December 2010.;

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

Not listed.

Seveso Directive

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
E1	environmental hazards (hazardous to the aquatic environment, cat. 1)	100	200	56)

Notation

56) Hazardous to the Aquatic Environment in category Acute 1 or Chronic 1

Deco-Paint Directive

VOC content	100 %
VOC content	1.000 g/l

Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	1.000 g/l

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

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Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not 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
TW	TCSI	substance is listed

Legend

TCSI Taiwan Chemical Substance Inventory

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-relevant
2.3	Endocrine disrupting properties: Does not contain an endocrine disruptor (EDC) in a concentration of $\geq 0,1\%$.	Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)

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Abbr.	Descriptions of used abbreviations
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
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
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.
Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

Disclaimer

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