

Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



Loganic acid ROTICHROM® HPLC

article number: **4158**
Version: **3.0 en**
Replaces version of: 2022-07-08
Version: (2)

date of compilation: 2019-04-08
Revision: 2024-03-04

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

1.1 Product identifier

| | |
|---------------------------------|-------------------------------------|
| Identification of the substance | Loganic acid ROTICHROM® HPLC |
| Article number | 4158 |
| EC number | 244-875-9 |
| CAS number | 22255-40-9 |

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 Service City Hospital | Dudley Rd | B187QH Birmingham | 844 892 0111 | |

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

This substance does not meet the criteria for classification.

2.2 Label elements

Labelling

not required

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2.3 Other hazards

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 | Loganic acid |
| Molecular formula | $C_{16}H_{24}O_{10}$ |
| Molar mass | 376,4 g/mol |
| CAS No | 22255-40-9 |
| EC No | 244-875-9 |

Impurities/additives/constituents:

| Name of substance | Identifier | Wt% |
|-------------------|---|-----|
| Acetonitrile | CAS No 75-05-8 EC No 200-835-2 Index No 608-001-00-3 | < 3 |

Remarks

For full text of abbreviations: see SECTION 16

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.

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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, foam, dry extinguishing powder, ABC-powder

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. 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

No special measures are necessary.

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. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically.

Other information relating to spills and releases

Place in appropriate containers for disposal.

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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.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. 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: 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.

| Relevant DNELs of components | | | | | | |
|------------------------------|---------|-----------|----------------------|------------------------------------|-------------------|----------------------------|
| Name of substance | CAS No | End-point | Threshold level | Protection goal, route of exposure | Used in | Exposure time |
| Acetonitrile | 75-05-8 | DNEL | 68 mg/m ³ | human, inhalatory | worker (industry) | chronic - systemic effects |
| Acetonitrile | 75-05-8 | DNEL | 68 mg/m ³ | human, inhalatory | worker (industry) | acute - systemic effects |
| Acetonitrile | 75-05-8 | DNEL | 68 mg/m ³ | human, inhalatory | worker (industry) | chronic - local effects |
| Acetonitrile | 75-05-8 | DNEL | 68 mg/m ³ | human, inhalatory | worker (industry) | acute - local effects |
| Acetonitrile | 75-05-8 | DNEL | 32,2 mg/kg bw/day | human, dermal | worker (industry) | chronic - systemic effects |

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| Relevant PNECs of components | | | | | | |
|------------------------------|---------|-----------|-----------------|-----------------------|------------------------------|------------------------------|
| Name of substance | CAS No | End-point | Threshold level | Organism | Environmental compartment | Exposure time |
| Acetonitrile | 75-05-8 | PNEC | 10 mg/l | aquatic organisms | freshwater | short-term (single instance) |
| Acetonitrile | 75-05-8 | PNEC | 1 mg/l | aquatic organisms | marine water | short-term (single instance) |
| Acetonitrile | 75-05-8 | PNEC | 32 mg/l | aquatic organisms | sewage treatment plant (STP) | short-term (single instance) |
| Acetonitrile | 75-05-8 | PNEC | 40,5 mg/kg | aquatic organisms | freshwater sediment | short-term (single instance) |
| Acetonitrile | 75-05-8 | PNEC | 4,05 mg/kg | aquatic organisms | marine sediment | short-term (single instance) |
| Acetonitrile | 75-05-8 | PNEC | 2,23 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.

• 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



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Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White).

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 | solid |
| Form | powder |
| Colour | whitish |
| Odour | odourless |
| Melting point/freezing point | 179 – 184 °C |
| 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 applicable |
| Auto-ignition temperature | not determined |
| Decomposition temperature | not relevant |
| pH (value) | not applicable |
| Kinematic viscosity | not relevant |
| <u>Solubility(ies)</u> | |
| Water solubility | not determined |
| <u>Partition coefficient</u> | |
| Partition coefficient n-octanol/water (log value): | -1,805 |
| Vapour pressure | not determined |
| <u>Density and/or relative density</u> | |
| Density | not determined |
| Relative vapour density | Information on this property is not available. |
| Particle characteristics | No data available. |
| <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

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

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

There are no specific conditions known which have to be avoided.

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

This substance does not meet the criteria for classification.

Acute toxicity

Shall not be classified as acutely toxic.

| Acute toxicity of components | | | | | |
|------------------------------|---------|----------------|----------|--------------|---------|
| Name of substance | CAS No | Exposure route | Endpoint | Value | Species |
| Acetonitrile | 75-05-8 | oral | LD50 | 469 mg/kg | mouse |
| Acetonitrile | 75-05-8 | dermal | LD50 | >2.000 mg/kg | rabbit |

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.

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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

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

Shall not be classified as hazardous to the aquatic environment.

| Aquatic toxicity (acute) of components | | | | | |
|--|---------|----------|------------|---------|---------------|
| Name of substance | CAS No | Endpoint | Value | Species | Exposure time |
| Acetonitrile | 75-05-8 | LC50 | 1.640 mg/l | fish | 96 h |
| Acetonitrile | 75-05-8 | ErC50 | 9.696 mg/l | algae | 72 h |

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Aquatic toxicity (chronic) of components

| Name of substance | CAS No | Endpoint | Value | Species | Exposure time |
|-------------------|---------|----------|-------------|----------------|---------------|
| Acetonitrile | 75-05-8 | EC50 | >1.000 mg/l | microorganisms | 30 min |

12.2 Persistence and degradability

Theoretical Oxygen Demand: 1,445 mg/mg
Theoretical Carbon Dioxide: 1,871 mg/mg

Degradability of components

| Name of substance | CAS No | Process | Degradation rate | Time | Method | Source |
|-------------------|---------|---------------------------|------------------|------|--------|--------|
| Acetonitrile | 75-05-8 | biotic/abiotic | 98 % | 28 d | | |
| Acetonitrile | 75-05-8 | carbon dioxide generation | 70 % | 21 d | | ECHA |

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

| | |
|---------------------------|--------|
| n-octanol/water (log KOW) | -1,805 |
|---------------------------|--------|

Bioaccumulative potential of components

| Name of substance | CAS No | BCF | Log KOW | BOD5/COD |
|-------------------|---------|-----|-----------------------------|----------|
| Acetonitrile | 75-05-8 | | -0,34 (pH value: ~7, 25 °C) | |

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.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

Sewage disposal-relevant information

Do not empty into drains.

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Waste treatment of containers/packagings

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.

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** not subject to transport regulations
- 14.2 UN proper shipping name** not assigned
- 14.3 Transport hazard class(es)** none
- 14.4 Packing group** not assigned
- 14.5 Environmental hazards** non-environmentally hazardous acc. to the dangerous goods regulations
- 14.6 Special precautions for user**
There is no additional information.
- 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**
- 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

Relevant provisions of the European Union (EU)

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 |
| | not assigned | | |

Deco-Paint Directive

| | |
|-------------|-----|
| VOC content | 0 % |
|-------------|-----|

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Industrial Emissions Directive (IED)

| | |
|-------------|-----|
| VOC content | 0 % |
|-------------|-----|

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

not listed

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

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

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 |
|---------|-----------|---------------------|
| EU | ECSI | substance is listed |
| TW | TCSI | substance is listed |
| VN | NCI | substance is listed |

Legend

ECSI EC Substance Inventory (EINECS, ELINCS, NLP)
NCI National Chemical Inventory
TCSI Taiwan Chemical Substance Inventory

15.2 Chemical safety assessment

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

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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 (ED) at a concentration of $\geq 0,1\%$. | yes |
| 14.8 | Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN. | | yes |
| 15.1 | | National inventories: change in the listing (table) | 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) |
| BCF | Bioconcentration factor |
| BOD | Biochemical Oxygen Demand |
| CAS | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances) |
| COD | Chemical oxygen demand |
| 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 |
| 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 |
| ErC50 | \equiv 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 |
| GB REACH | The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended) |
| 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 |
| index No | The Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008 |

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| Abbr. | Descriptions of used abbreviations |
|---------|---|
| 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 |
| log KOW | n-Octanol/water |
| NLP | No-Longer Polymer |
| PBT | Persistent, Bioaccumulative and Toxic |
| PNEC | Predicted No-Effect Concentration |
| 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) |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and very Bioaccumulative |

Key literature references and sources for data

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).

Disclaimer

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