

Loganic acid ROTICHROM® HPLC

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

Product identifier 1.1

Identification of the substance

Article number

Registration number (REACH)

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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 CAS number 244-875-9 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 Department Health, Safety and Environment sheet:

e-mail (competent person):

sicherheit@carlroth.de

Emergency telephone number 1.4

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

This substance does not meet the criteria for classification in accordance with Regulation No 1272/ 2008/EC.

2.2 Label elements

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

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 $\ge 0,1\%$.

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	<3
	EC No 200-835-2	
	Index No 608-001-00-3	

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 sub- stance	CAS No	End- point	Threshol d level	Protection goal, route of exposure	Used in	Exposure time
Acetonitrile	75-05-8	DNEL	68 mg/m ³	human, inhalat- ory	worker (industry)	chronic - systemic effects
Acetonitrile	75-05-8	DNEL	68 mg/m ³	human, inhalat- ory	worker (industry)	acute - systemic effects
Acetonitrile	75-05-8	DNEL	68 mg/m ³	human, inhalat- ory	worker (industry)	chronic - local ef- fects
Acetonitrile	75-05-8	DNEL	68 mg/m ³	human, inhalat- ory	worker (industry)	acute - local ef- fects
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 sub- stance	CAS No	End- point	Threshol d level	Organism	Environmental compartment	Exposure time
Acetonitrile	75-05-8	PNEC	10 ^{mg} / _l	aquatic organ- isms	freshwater	short-term (single instance)
Acetonitrile	75-05-8	PNEC	1 ^{mg} / _l	aquatic organ- isms	marine water	short-term (single instance)
Acetonitrile	75-05-8	PNEC	32 ^{mg} / _l	aquatic organ- isms	sewage treatment plant (STP)	short-term (single instance)
Acetonitrile	75-05-8	PNEC	40,5 ^{mg} / _{kg}	aquatic organ- isms	freshwater sedi- ment	short-term (single instance)
Acetonitrile	75-05-8	PNEC	4,05 ^{mg} / _{kg}	aquatic organ- isms	marine sediment	short-term (single instance)
Acetonitrile	75-05-8	PNEC	2,23 ^{mg} / _{kg}	terrestrial organ- isms	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

Information on basic physical and chemical properties Physical state solid Form powder Colour whitish Odour odourless 179 - 184 °C Melting point/freezing point Boiling point or initial boiling point and boiling not determined range this material is combustible, but will not ignite Flammability 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 Solubility(ies) not determined Water solubility Partition coefficient Partition coefficient n-octanol/water (log value): -1,805 Vapour pressure not determined Density and/or relative density Density not determined Relative vapour density Information on this property is not available. Particle characteristics No data available. Other safety parameters Oxidising properties none



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9.2 Other information

Information with regard to physical hazard classes:

Other safety characteristics:

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

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 hazard classes as defined in Regulation (EC) No 1272/2008

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

This substance does not meet the criteria for classification in accordance with Regulation No 1272/ 2008/EC.

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.



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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).

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 $\ge 0,1\%$.

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 sub- stance	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 sub- stance	CAS No	Endpoint	Value	Species	Exposure time
Acetonitrile	75-05-8	EC50	>1.000 ^{mg} / _l	microorganisms	30 min

12.2 Persistence and degradability

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Theoretical Oxygen Demand: 1,445 <sup>mg</sup>/<sub>mg</sub>
Theoretical Carbon Dioxide: 1,871 <sup>mg</sup>/<sub>mg</sub>
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Degradability of components						
Name of substance	CAS No	Process	Degrada- tion 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 $\ge 0,1\%$.
- 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

14.2 UN proper shipping name

14.3 Transport hazard class(es)

14.4 Packing group

14.5 Environmental hazards

not subject to transport regulations

not assigned

none

not assigned

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)

Restrictions according to REACH, Annex XVII not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list Not listed.



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Seveso	Directive						
2012/18/EU (Seveso III)							
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the ap- plication of lower and upper-tier re- quirements	Notes				
	not assigned						

Deco-Paint Directive

VOC content	0 %
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Industrial Emissions Directive (IED)

VOC content	0 %
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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

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 NCI

EC Substance Inventory (EINECS, ELINCS, NLP) National Chemical Inventory



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Legend TCSI Taiwan Chemical Substance Inventory

15.2 Chemical safety assessment

No Chemical Safety Assessment has been carried out for this substance. According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.

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
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional in- formation: Not subject to ADR, RID and ADN.		yes
15.1		National inventories: change in the listing (table)	yes
15.2	Chemical Safety Assessment: No Chemical Safety Assessment has been car- ried out for this substance.	Chemical safety assessment: No Chemical Safety Assessment has been car- ried out for this substance. According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or compon- ents of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concern- ing 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)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
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 identi- fier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor



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Abbr.	Descriptions of used abbreviations
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
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 Na- tions
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
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
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). 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.