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Loganic acid ROTICHROM® HPLC

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

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

1.1 Product identifier

Identification of the substance

Article number

CAS number

Loganic acid ROTICHROM® HPLC

4158

22255-40-9

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

Relevant identified uses:

Uses advised against:

Laboratory chemical Laboratory and analytical use

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

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

This substance does not meet the criteria for classification.

2.2 Label elements

Labelling

not required

10: +49(0)/21-56060	
+49 (0) 721 - 56 06 149	
icherheit@carlroth.de	
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acc. to Safe Work Australia - Code of Practice

Loganic acid ROTICHROM® HPLC

article number: 4158

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

Impurities/additives/constituents:

Name of substance	Identifier	Wt%
Acetonitrile	CAS No 75-05-8	<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.

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



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Loganic acid ROTICHROM® HPLC

article number: 4158

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.

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.

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Loganic acid ROTICHROM® HPLC

article number: 4158

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		

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)

acc. to Safe Work Australia - Code of Practice



Loganic acid ROTICHROM® HPLC

article number: 4158

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	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



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.

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Loganic acid ROTICHROM® HPLC

article number: 4158

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				
	Solubility(ies)					
	Water solubility	not determined				
	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				
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.				

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Loganic acid ROTICHROM® HPLC

article number: 4158

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.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

acc. to Safe Work Australia - Code of Practice

Loganic acid ROTICHROM® HPLC

article number: 4158



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 $\ge 0,1\%$.

SECTION 12: Ecological information

12.1 Toxicity

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

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

Theoretical Oxygen Demand: 1.445 $^{\rm mg}/_{\rm mg}$ Theoretical Carbon Dioxide: 1.871 $^{\rm mg}/_{\rm mg}$

acc. to Safe Work Australia - Code of Practice



Loganic acid ROTICHROM® HPLC

article number: 4158

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.

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.

acc. to Safe Work Australia - Code of Practice

Loganic acid ROTICHROM® HPLC

article number: 4158

SECTION 14: Transport information

- 14.1 UN 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

not assigned

not assigned

non-environmentally hazardous acc. to the dangerous 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.

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

15.2 Chemical Safety Assessment

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



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Loganic acid ROTICHROM® HPLC

article number: 4158

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		
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		
ED	Endocrine disruptor		
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 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		
log KOW	n-Octanol/water		
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		

Loganic acid ROTICHROM® HPLC



article number: 4158

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).

Disclaimer

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