

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description:	<u>D(-)-Quinic acid</u>
Cat No. :	160500000; 160500250; 160501000; 160505000
Synonyms	1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid
CAS No	77-95-2
EC No	201-072-8
Molecular Formula	C7 H12 O6
REACH registration number	01-2120104723-67

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

Recommended Use	Laboratory chemicals.
Sector of use	SU3 - Industrial uses: Uses of substances as such or in preparations at industrial sites
Product category	PC21 - Laboratory chemicals
Process categories	PROC15 - Use as a laboratory reagent
Environmental release category	ERC6a - Industrial use resulting in manufacture of another substance (use of intermediates)
Uses advised against	No Information available

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name
Fisher Scientific UK
Bishop Meadow Road,
Loughborough, Leicestershire LE11 5RG, United Kingdom

EU entity/business name
Thermo Fisher Scientific
Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

E-mail address begin.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

Based on available data, the classification criteria are not met

Health hazards

Serious Eye Damage/Eye Irritation

Category 2 (H319)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H319 - Causes serious eye irritation

Precautionary Statements

P280 - Wear eye protection/ face protection
P264 - Wash face, hands and any exposed skin thoroughly after handling
P337 + P313 - If eye irritation persists: Get medical advice/attention

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]-	77-95-2	EEC No. 201-072-8	> 95	Eye Irrit. 2 (H319)

REACH registration number

01-2120104723-67

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

ACR16050

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

4.1. Description of first aid measures

General Advice	If symptoms persist, call a physician.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Self-Protection of the First Aider	No special precautions required.

4.2. Most important symptoms and effects, both acute and delayed

No information available.

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂).

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

6.2. Environmental precautions

Should not be released into the environment.

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 11
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

See values below.

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]-77-95-2 (> 95)	PNEC = 0.116mg/L	PNEC = 0.0989mg/kg sediment dw	PNEC = 1.16mg/L		PNEC = 0.0987mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]-77-95-2 (> 95)	PNEC = 0.0116mg/L	PNEC = 0.00989mg/kg sediment dw			

8.2. Exposure controls

Engineering Measures

None under normal use conditions. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal protective equipment

Eye Protection

Wear safety glasses with side shields (or goggles) Goggles (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Butyl rubber				
Nitrile rubber				
Neoprene				
PVC				

Skin and body protection

Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection

No protective equipment is needed under normal use conditions.

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Particle filter

Small scale/Laboratory use

Maintain adequate ventilation

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

Environmental exposure controls

No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

9.1. Information on basic physical and chemical properties

Physical State	Powder Solid	
Appearance	White	
Odor	Odorless	
Odor Threshold	No data available	
Melting Point/Range	166 - 168 °C / 330.8 - 334.4 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	No information available	Method - No information available
Autoignition Temperature	Not applicable	
Decomposition Temperature	No data available	
pH	> 2	
Viscosity	Not applicable	Solid
Water Solubility	400 g/L (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]	- 2.45	
-		
Vapor Pressure	No information available	
Density / Specific Gravity	1.64	
Bulk Density	No data available	
Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

9.2. Other information

Molecular Formula	C7 H12 O6
Molecular Weight	192.17
Evaporation Rate	Not applicable - Solid

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity
None known, based on information available

10.2. Chemical stability
No information available.

10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid
Incompatible products.

10.5. Incompatible materials
Oxidizing agent.

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information	No acute toxicity information is available for this product
(a) acute toxicity;	
Oral	Based on available data, the classification criteria are not met
Dermal	Based on available data, the classification criteria are not met
Inhalation	Based on available data, the classification criteria are not met
(b) skin corrosion/irritation;	Based on available data, the classification criteria are not met
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization;	
Respiratory	Based on available data, the classification criteria are not met
Skin	Based on available data, the classification criteria are not met
(e) germ cell mutagenicity;	Based on available data, the classification criteria are not met
(f) carcinogenicity;	Based on available data, the classification criteria are not met There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	Based on available data, the classification criteria are not met
(h) STOT-single exposure;	Based on available data, the classification criteria are not met
(i) STOT-repeated exposure;	Based on available data, the classification criteria are not met
Target Organs	None known.
(j) aspiration hazard;	Not applicable Solid
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects,both acute and delayed	No information available.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

12.1. Toxicity

Ecotoxicity effects

12.2. Persistence and degradability

Persistence

Soluble in water, Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]-	- 2.45	No data available

12.4. Mobility in soil

The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

**Persistent Organic Pollutant
Ozone Depletion Potential**

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Solutions with low pH-value must be neutralized before discharge.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

Not regulated

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

- 14.1. UN number
- 14.2. UN proper shipping name
- 14.3. Transport hazard class(es)
- 14.4. Packing group

ADR Not regulated

- 14.1. UN number
- 14.2. UN proper shipping name
- 14.3. Transport hazard class(es)
- 14.4. Packing group

IATA Not regulated

- 14.1. UN number
- 14.2. UN proper shipping name
- 14.3. Transport hazard class(es)
- 14.4. Packing group

- 14.5. Environmental hazards No hazards identified
- 14.6. Special precautions for user No special precautions required.
- 14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.b eta.)]-	77-95-2	201-072-8	-	-	X	X	KE-33516	-	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.b eta.)]-	77-95-2	-	-	-	X	X	X	-

Legend: X - Listed '-' - Not Listed **KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-,	77-95-2	-	-	-

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

[1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]-				
--	--	--	--	--

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]-	77-95-2	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification

See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]-	WGK1	

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H319 - Causes serious eye irritation

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

SAFETY DATA SHEET

D(-)-Quinic acid

Revision Date 22-Sep-2023

IECSC - Chinese Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances

AICS - Australian Inventory of Chemical Substances
NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit
ACGIH - American Conference of Governmental Industrial Hygienists
DNEL - Derived No Effect Level
RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOEC - No Observed Effect Concentration
PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average
IARC - International Agency for Research on Cancer
Predicted No Effect Concentration (PNEC)
LD50 - Lethal Dose 50%
EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water
vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road
IMO/MDG - International Maritime Organization/International Maritime Dangerous Goods Code
OECD - Organisation for Economic Co-operation and Development
BCF - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
MARPOL - International Convention for the Prevention of Pollution from Ships
ATE - Acute Toxicity Estimate
VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Creation Date 10-Feb-2011
Revision Date 22-Sep-2023
Revision Summary SDS sections updated: 2, 3.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet