

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: Quinic acid

Date of issue: 07.12.2012

Revision date: 15.02.2024

Version: 11

Replaces version: 10

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

1.1. Product identifier

Product form : Substance
Substance name : Quinic acid
Chemical name : 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid
IUPAC name : (1S, 3R, 4S, 5R)- 1,3,4,5-Tetrahydroxy-cyclohexanecarboxylic acid
EC No : 201-072-8
CAS No : 77-95-2
REACH registration No : 01-2120104723-67-xxxx
Formula : C7H12O6

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

1.2.1. Relevant identified uses

Main use category : Industrial use. Professional use
Use of the substance/mixture : Intermediate
Laboratory chemicals
Other dielectric material
Pharmaceuticals
Food additive

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Manufacturer/Supplier

Buchler GmbH
Harxbuetteler Straße 3
38110 Braunschweig - Germany
T +49 5307 9310
info@buchler-gmbh.com - www.buchler-gmbh.com

Safety data sheet: DLAC Dienstleistungsgagentur Chemie GmbH, E-Mail: sds@dlac-gmbh.de

1.4. Emergency telephone number

Country	Organisation/Company	Address	Emergency number
Germany	Giftinformationszentrum-Nord Zentrum Pharmakologie und Toxikologie der Universität Göttingen	Robert-Koch-Straße 40 D-37075 Göttingen	+49 551 19240 (German/English)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

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

Serious eye damage/eye irritation, Category 2 H319

Full text of H statements: see section 16

Adverse physicochemical, human health and environmental effects

Causes serious eye irritation.

2.2. Label elements

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

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H319 - Causes serious eye irritation.

Precautionary statements (CLP) :

P264 - Wash hands thoroughly after handling.
P280 - Wear protective gloves, protective clothing, eye protection.
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove

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contact lenses, if present and easy to do. Continue rinsing.
P337+P313 - If eye irritation persists: Get medical advice/attention.

2.3. Other hazards

Contains no substance(s) included in the list established in accordance with Article 59(1) of REACH for having endocrine disrupting properties, or is not identified as having endocrine disrupting properties in accordance with the criteria set out in Commission Delegated Regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605.

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance name : Quinic acid

EC No : 201-072-8

CAS No : 77-95-2

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
Quinic acid	(CAS No) 77-95-2 (EC No) 201-072-8 (REACH No) 01-2120104723-67-xxxx	≥ 98.0	Eye Irrit. 2, H319

Full text of H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : Get medical advice/attention if you feel unwell. If possible show him this sheet. Failing this, show him the packaging or label. Never give anything by mouth to an unconscious person. Place the affected person in the recovery position.

First-aid measures after inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing.

First-aid measures after skin contact : Take off immediately all contaminated clothing and wash it before reuse. Wash with plenty of soap and water.

First-aid measures after eye contact : IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.

First-aid measures after ingestion : Rinse mouth. Drink plenty of water as a precaution.

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

Symptoms/injuries after eye contact : Causes serious eye irritation.

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

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Adapt extinguishing agent to suit the environment. Water spray. Foam. Carbon dioxide. Dry extinguishing powder.

Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Hazardous decomposition products in case of fire : Carbon oxides (CO, CO₂).

5.3. Advice for firefighters

Firefighting instructions : Use water spray or fog for cooling exposed containers. Prevent fire-fighting water from entering environment.

Protection during firefighting : Use a self-contained breathing apparatus and also a protective suit (EN 469).

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Stop leak if safe to do so. Provide adequate ventilation. Avoid contact with skin and eyes. Do not breathe dust.

6.1.1. For non-emergency personnel

Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

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6.1.2. For emergency responders

Protective equipment : Use personal protective equipment as required. Wear suitable respiratory equipment in case of insufficient ventilation.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if substance enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Take up mechanically (sweeping, shovelling) and collect in suitable container for disposal. Minimize generation of dust. Dispose of in accordance with relevant local regulations.

6.4. Reference to other sections

Concerning personal protective equipment to use, see section 8. Concerning disposal elimination after cleaning, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Provide local exhaust or general room ventilation. Avoid dust formation. Avoid contact with skin and eyes. Keep container closed when not in use.

Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. When using do not eat, drink or smoke. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Take off contaminated clothing and wash it before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store in original container. Store tightly closed in a dry and cool place. Keep out of direct sunlight. Protect from moisture.

Storage temperature : 15 - 30 °C

Prohibitions on mixed storage : Keep away from food, drink and animal feedingstuffs.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Quinic acid (77-95-2)	
PNEC (Water)	
PNEC aqua (freshwater)	0.116 mg/l
PNEC aqua (marine water)	0.0116 mg/l
PNEC aqua (intermittent, freshwater)	1.16 mg/l
PNEC (Sediment)	
PNEC sediment (freshwater)	0.0989 mg/kg dwt
PNEC sediment (marine water)	0.00989 mg/kg dwt
PNEC (Soil)	
PNEC soil	0.0987 mg/kg dwt

8.2. Exposure controls

Appropriate engineering controls:

Use adequate ventilation. Avoid dust formation.

Hand protection:

Wear suitable gloves (EN 374). Latex. Nitrile rubber. Butyl rubber. 0.4 mm. The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed

Eye protection:

Chemical goggles or safety glasses (EN 166).

Skin and body protection:

Wear suitable protective clothing (EN 344).

Respiratory protection:

Where exposure through inhalation may occur from use, respiratory protection is recommended. Dust production: dust mask with filter type P2

Environmental exposure controls:

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Avoid release to the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid, powder
Colour	: White
Odour	: Odourless
Melting point/freezing point	: 162 - 166 °C
Boiling point or initial boiling point and boiling range	: No data available
Flammability	: No data available
Lower and upper explosion limit	: No data available
Flash point	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
pH	: > 2.0
Kinematic viscosity	: Not applicable
Solubility	: Water: 400 g/l
Partition coefficient n-octanol/water (log value)	: -2.45
Vapour pressure	: No data available
Density and/or relative density	: 1.637 g/cm ³
Relative vapour density	: No data available
Particle characteristics	: No data available

9.2. Other information

Molecular mass	: 192.2 g/mol
Minimum ignition energy	: 100 - 300 mJ
Bulk density	: 670 - 750 kg/m ³
Explosive properties	: The substance is not explosive. Dust can form an explosive mixture with air.
Oxidising properties	: The substance has no oxidising properties

SECTION 10: Stability and reactivity

10.1. Reactivity

No dangerous reactions known under normal conditions of use.

10.2. Chemical stability

Stable under use and storage conditions as recommended in section 7 for a minimum of 5 years.

10.3. Possibility of hazardous reactions

None under normal use.

10.4. Conditions to avoid

Direct sunlight. High temperature. Quinic acid lactone and aromatic phenols are formed.

10.5. Incompatible materials

Oxidizing agents.

10.6. Hazardous decomposition products

In case of fire: Carbon monoxide. Carbon dioxide.

SECTION 11: Toxicological information

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

Acute toxicity	: Not classified Based on available data, the classification criteria are not met
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Quinic acid (77-95-2)

LD50 oral rat	3265 mg/kg (Cyclohexanecarboxylic acid)
Skin corrosion/irritation	: Not classified Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Causes serious eye irritation.

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Respiratory or skin sensitisation	: Not classified Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified Based on available data, the classification criteria are not met
Specific target organ toxicity (single exposure)	: Not classified Based on available data, the classification criteria are not met
Specific target organ toxicity (repeated exposure)	: Not classified Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified Based on available data, the classification criteria are not met

11.2. Information on other hazards

11.2.1. Endocrine disrupting properties

Endocrine disruption for human health : The substance/mixture has no endocrine disrupting properties.

11.2.2. Other information

Potential adverse human health effects and symptoms : Based on available data, the classification criteria are not met

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity : Not classified
Chronic aquatic toxicity : Not classified

Quinic acid (77-95-2)	
LC50 fish	> 100 mg/l 96 h (Shikimic acid)
EC50 daphnia	> 5 g/l 48 h, Daphnia magna
NOEC chronic crustacea	> 5 g/l 48 h, Daphnia magna
NOEC chronic algae	> 10 mg/l 10 d, Microcystis aeruginosa

12.2. Persistence and degradability

Quinic acid (77-95-2)	
Persistence and degradability	Readily biodegradable.
Biodegradation	89.7 % 29 d (OECD 301 B)

12.3. Bioaccumulative potential

Quinic acid (77-95-2)	
Bioconcentration factor (BCF REACH)	3.16
Log Pow	-2.45
Bioaccumulative potential	Low bioaccumulation potential.

12.4. Mobility in soil

Quinic acid (77-95-2)	
Log Koc	-2.02 - 1

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT- or vPvB criteria of REACH regulation, annex XIII.

12.6. Endocrine disrupting properties

Endocrine disruption for the environment : The substance/mixture has no endocrine disrupting properties.

12.7. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste) : Dispose in a safe manner in accordance with local/national regulations.

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Waste treatment methods	: This material and its container must be disposed of as hazardous waste. Do not dispose of with domestic waste. Do not empty into drains.
Waste disposal recommendations	: Empty the packaging completely prior to disposal. When totally empty, containers are recyclable like any other packing.
European List of Waste (LoW) code	: 07 00 00 - WASTES FROM ORGANIC CHEMICAL PROCESSES 07 01 00 - wastes from the manufacture, formulation, supply and use (MFSU) of basic organic chemicals
Waste code	: The waste code number according to the Ordinance on the European Waste Catalogue (EWC) depends on the waste producer and can therefore vary for any given product. The waste code number is therefore to be gleaned separately from each waste producer.

SECTION 14: Transport information

In accordance with ADR / IMDG / IATA

14.1. UN number or ID number

UN-No. (ADR)	: Not applicable
UN-No. (IMDG)	: Not applicable
UN-No. (IATA)	: Not applicable

14.2. UN proper shipping name

Proper Shipping Name (ADR)	: Not applicable
Proper Shipping Name (IMDG)	: Not applicable
Proper Shipping Name (IATA)	: Not applicable

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR)	: Not applicable
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IMDG

Transport hazard class(es) (IMDG)	: Not applicable
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IATA

Transport hazard class(es) (IATA)	: Not applicable
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14.4. Packing group

Packing group (ADR)	: Not applicable
Packing group (IMDG)	: Not applicable
Packing group (IATA)	: Not applicable

14.5. Environmental hazards

Dangerous for the environment	: No
Marine pollutant	: No
Other information	: No supplementary information available

14.6. Special precautions for user

- Overland transport

Not applicable

- Transport by sea

Not applicable

- Air transport

Not applicable

14.7. Maritime transport in bulk according to IMO instruments

Not applicable

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SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

REACH Annex XIV (Authorisation List)

Contains no substance(s) listed on REACH Annex XIV (Authorisation List).

REACH Candidate List (SVHC)

Contains no substance(s) listed on the REACH Candidate List.

PIC Regulation (Prior Informed Consent)

Contains no substance(s) listed on the PIC list (Regulation EU 649/2012 concerning the export and import of hazardous chemicals).

POP Regulation (Persistent Organic Pollutants)

Contains no substance(s) listed on the POP list (Regulation EU 2019/1021 on persistent organic pollutants).

Ozone Regulation (1005/2009)

Contains no substance(s) listed on the Ozone Depletion list (Regulation EU 1005/2009 on substances that deplete the ozone layer).

Explosives Precursors Regulation (2019/1148)

Contains no substance(s) listed on the Explosives Precursors list (Regulation EU 2019/1148 on the marketing and use of explosives precursors).

Drug Precursors Regulation (273/2004)

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances).

15.1.2. National regulations

No additional information available

15.2. Chemical safety assessment

For this substance a chemical safety assessment was not carried out.

SECTION 16: Other information

Data source : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Changes compared to earlier Versions : Section 2.3. Other hazards
Section 11.2.1 Endocrine disrupting properties
Section 12.6. Endocrine disrupting properties
Section 15.1.1. EU-Regulations

Review : -

Abbreviations and acronyms:

ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EC50	The effective concentration of substance that causes 50 % of the maximum response (Median Effective Concentration)
IATA	International Air Transport Association
IMDG	"International Maritime Dangerous Goods Code" for the transport of dangerous goods by sea
LC50	Lethal Concentration to 50 % of a test population (Median Lethal Concentration)
LD50	Lethal Dose to 50 % of a test population (Median Lethal Dose)
LOAEL	Lowest Observed Adverse Effect Level
NOAEC/L	No Observed Adverse Effect Concentration/Level
NOEC/L	No Observed Effect Concentration/Level
OECD	Organisation for Economic Cooperation and Development
PBT	Persistent, Bioaccumulative and Toxic substance
PNEC	Predicted No-Effect Concentration
REACH	Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals

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RID	Regulation concerning the International Carriage of Dangerous Goods by Rail
SDS	Safety Data Sheet
STP	Sewage Treatment Plant
UFI	Unique Formula Identifier
vPvB	Very Persistent and Very Bioaccumulative

Full text of H- and EUH-statements:

Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
H319	Causes serious eye irritation.

SDS EU (REACH Annex II)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.