

Safety data sheet

Safe Work Australia - Code of Practice



Acetonitrile $\geq 99,5\%$, for synthesis

article number: **4380**
Version: **GHS 3.0 en**
Replaces version of: 2018-05-30
Version: (GHS 2)

date of compilation: 2016-11-04
Revision: 2020-09-03

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

1.1 Product identifier

Identification of the substance	Acetonitrile $\geq 99,5\%$, for synthesis
Article number	4380
Registration number (REACH)	01-2119471307-38-xxxx
Index No	608-001-00-3
EC number	200-835-2
CAS number	75-05-8

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

Identified uses: laboratory chemical
laboratory and analytical use

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
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

Emergency information service

Poison Centre Munich: +49/(0)89 19240

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

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Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
2.6	flammable liquid	(Flam. Liq. 2)	H225
3.1O	acute toxicity (oral)	(Acute Tox. 4)	H302
3.1D	acute toxicity (dermal)	(Acute Tox. 4)	H312
3.1I	acute toxicity (inhal.)	(Acute Tox. 4)	H332
3.3	serious eye damage/eye irritation	(Eye Irrit. 2)	H319

2.2 Label elements

Labelling GHS

Signal word

Danger

Pictograms

GHS02, GHS07



Hazard statements

H225 Highly flammable liquid and vapour
H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled
H319 Causes serious eye irritation

Precautionary statements

Precautionary statements - prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P233 Keep container tightly closed.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves/protective clothing.

Precautionary statements - response

P302+P352 IF ON SKIN: Wash with plenty of soap and water.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P312 Call a POISON CENTER or doctor/physician if you feel unwell.
P370+P378 In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction.

Precautionary statements - storage

P403+P235 Store in a well-ventilated place. Keep cool.

Precautionary statements - disposal

P501 Dispose of contents/container to industrial combustion plant.

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

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Symbol(s)



2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Acetonitrile
Index No	608-001-00-3
Registration number (REACH)	01-2119471307-38-xxxx
EC number	200-835-2
CAS number	75-05-8
Molecular formula	C_2H_3N
Molar mass	41.05 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

After eye contact: Irritant effects, Conjunctival redness of the eyes,
Following skin contact: Localised redness, oedema, pruritis and/or pain,
Following ingestion: Vomiting, Irritation, Headaches and dizziness may occur,
Following inhalation: Cough, pain, choking, and breathing difficulties

4.3 Indication of any immediate medical attention and special treatment needed

none

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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours can form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: nitrogen oxides (NO_x), carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

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

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Explosive properties.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

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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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

- **Measures to prevent fire as well as aerosol and dust generation**



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

Ground/bond container and receiving equipment.

- **Ventilation requirements**

Use local and general ventilation.

- **Specific designs for storage rooms or vessels**

Recommended storage temperature: 15 – 25 °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)

Country	Name of agent	CAS No	Notation	Identifier	TWA [ppm]	TWA [mg/m ³]	STEL [ppm]	STEL [mg/m ³]	Ceiling-C [ppm]	Ceiling-C [mg/m ³]	Source
AU	acetonitrile	75-05-8		WES	40	67	60	101			WES

Notation

Ceiling-C
STEL

Ceiling value is a limit value above which exposure should not occur
Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA

Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

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Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	68 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	68 mg/m ³	human, inhalatory	worker (industry)	acute - systemic effects
DNEL	68 mg/m ³	human, inhalatory	worker (industry)	chronic - local effects
DNEL	68 mg/m ³	human, inhalatory	worker (industry)	acute - local effects
DNEL	32.2 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

• environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	10 mg/l	freshwater	short-term (single instance)
PNEC	1 mg/l	marine water	short-term (single instance)
PNEC	32 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	7.53 mg/kg	freshwater sediment	short-term (single instance)
PNEC	2.41 mg/kg	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. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

Butyl caoutchouc (butyl rubber)

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- **material thickness**

0,5 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.

Flame-retardant protective clothing.

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of $> 65\text{ }^{\circ}\text{C}$, colour code: Brown).

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

Appearance

Physical state	liquid (fluid)
Colour	colourless
Odour	characteristic mild sweet
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	$-45,7\text{ }^{\circ}\text{C}$
Initial boiling point and boiling range	$81,6\text{ }^{\circ}\text{C}$ at 1,013 hPa
Flash point	$12,8\text{ }^{\circ}\text{C}$
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
<u>Explosive limits</u>	
• lower explosion limit (LEL)	4.4 vol% (50 g/m ³)
• upper explosion limit (UEL)	16 vol% (274 g/m ³)
Explosion limits of dust clouds	not relevant
Vapour pressure	94.51 hPa at $20\text{ }^{\circ}\text{C}$
Density	0.782 g/cm ³ at $20\text{ }^{\circ}\text{C}$
Vapour density	1.42 (air = 1)
Bulk density	Not applicable

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Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	1,000 g/l at 25 °C
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	-0.34
Soil organic carbon/water (log KOC)	0.654 (ECHA)
Auto-ignition temperature	524 °C - ECHA 524 °C
Decomposition temperature	no data available
Viscosity	
• kinematic viscosity	0.4987 mm ² /s at 20 °C
• dynamic viscosity	0.39 mPa s at 20 °C
Explosive properties	Shall not be classified as explosive
Oxidising properties	none
9.2 Other information	
Refractive index	1.344

SECTION 10: Stability and reactivity

10.1 Reactivity

Risk of ignition. Vapours can form explosive mixtures with air.

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: Peroxides, Strong oxidiser, Strong acid

10.4 Conditions to avoid

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

10.5 Incompatible materials

Rubber articles

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Exposure route	Endpoint	Value	Species	Source
oral	LD50	469 mg/kg	mouse	ECHA
dermal	LD50	>2,000 mg/kg	rabbit	ECHA

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Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor 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**

nausea, vomiting, dizziness

- **If in eyes**

slightly irritant but not relevant for classification

- **If inhaled**

cough, pain, choking, and breathing difficulties

- **If on skin**

Prolonged or repeated contact with skin or mucous membrane result in irritation symptoms such as redness, blistering, dermatitis, etc

Other information

None

SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
LC50	1,640 mg/l	fish	ECHA	96 h
ErC50	9,696 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
NOEC	102 mg/l	fish	ECHA	21 d

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12.2 Process of degradability

Not readily biodegradable. Theoretical Oxygen Demand with nitrification: 2.923 mg/mg
Theoretical Oxygen Demand: 1.559 mg/mg
Theoretical Carbon Dioxide: 2.144 mg/mg

Process	Degradation rate	Time
biotic/abiotic	98 %	28 d
carbon dioxide generation	70 %	21 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW) -0.34

12.4 Mobility in soil

Henry's law constant 3.5 Pa m³/mol at 20 °C

The Organic Carbon normalised adsorption coefficient 0.654

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

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.

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SECTION 14: Transport information

14.1	UN number	1648
14.2	UN proper shipping name Hazardous ingredients	ACETONITRILE Acetonitrile
14.3	Transport hazard class(es)	
	Class	3 (flammable liquids)
14.4	Packing group	II (substance presenting medium danger)
14.5	Environmental hazards	none (non-environmentally hazardous acc. to the dangerous goods regulations)
14.6	Special precautions for user	
	Provisions for dangerous goods (ADR) should be complied within the premises.	
14.7	Transport in bulk according to Annex II of MARPOL and the IBC Code	
	The cargo is not intended to be carried in bulk.	
14.8	Information for each of the UN Model Regulations	
	• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)	
	UN number	1648
	Proper shipping name	ACETONITRILE
	Particulars in the transport document	UN1648, ACETONITRILE, 3, II, (D/E)
	Class	3
	Classification code	F1
	Packing group	II
	Danger label(s)	3
		
	Excepted quantities (EQ)	E2
	Limited quantities (LQ)	1 L
	Transport category (TC)	2
	Tunnel restriction code (TRC)	D/E
	Hazard identification No	33
	Emergency Action Code	2YE
	• International Maritime Dangerous Goods Code (IMDG)	
	UN number	1648
	Proper shipping name	ACETONITRILE
	Particulars in the shipper's declaration	UN1648, ACETONITRILE, 3, II, 12.8°C c.c.

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Class	3
Marine pollutant	-
Packing group	II
Danger label(s)	3



• International Civil Aviation Organization (ICAO-IATA/DGR)

UN number	1648
Proper shipping name	Acetonitrile
Particulars in the shipper's declaration	UN1648, Acetonitrile, 3, II
Class	3
Packing group	II
Danger label(s)	3



SECTION 15: Regulatory information

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

National inventories

Substance is listed in the following national inventories:

Country	National inventories	Status
AU	AICS	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed

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Country	National inventories	Status
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

AICS	Australian Inventory of Chemical Substances
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

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

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1		Classification acc. to GHS: change in the listing (table)	yes
2.2		Pictograms: change in the listing (table)	yes
2.2		Hazard statements: change in the listing (table)	yes
2.2		Precautionary statements - prevention: change in the listing (table)	yes
2.2		Precautionary statements - response: change in the listing (table)	yes
2.2		Precautionary statements - storage: change in the listing (table)	yes
2.2		Precautionary statements - disposal	yes
2.2		Precautionary statements - disposal: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
8.1		• environmental values: change in the listing (table)	yes
14.8	Special provisions (SP): -		yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	ceiling value
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
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
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
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
NOEC	No Observed Effect Concentration
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

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Abbr.	Descriptions of used abbreviations
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
STEL	short-term exposure limit
TWA	time-weighted average
vPvB	very Persistent and very Bioaccumulative
WES	Safe Work Australia: Workplace exposure standards for airborne conatminants

Key literature references and sources for data

- UN Recommendations on the Transport of Dangerous Good
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
H225	highly flammable liquid and vapour
H302	harmful if swallowed
H312	harmful in contact with skin
H319	causes serious eye irritation
H332	harmful if inhaled

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.