

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**
Version: **3.0 en**
Replaces version of: 2016-11-04
Version: (2)

date of compilation: 2015-10-20
Revision: 2018-05-30

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

1.1 Product identifier

Identification of the substance	Acetonitrile
Article number	HN40
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
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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

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

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

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

2.2 Label elements

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

Signal word

Danger

Pictograms



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, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280 Wear protective gloves/eye protection.

Precautionary statements - response

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Precautionary statements - storage

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

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

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 ₂ H ₃ N
Molar mass	41,05 g/mol

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: HN40

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,
After 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

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)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

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

Advices on how to contain a spill

Covering of drains.

Advices on how to clean up a spill

Absorb with liquid-binding material (e.g. 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.

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

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

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]	Source
EU	acetonitrile	75-05-8		IOELV	40	70			2017/2398/EU
GB	acetonitrile	75-05-8		WEL	40	68	60	102	EH40/2005

Notation

STEL 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)

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	water	intermittent release
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)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

Endpoint	Threshold level	Environmental compartment	Exposure time
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.

• type of material

Butyl caoutchouc (butyl rubber)

• 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 °C, colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

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 °C
Initial boiling point and boiling range	81,6 °C at 1.013 hPa
Flash point	12,8 °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 °C
Density	0,782 g/cm ³ at 20 °C
Vapour density	1,42 (air = 1)
Bulk density	Not applicable
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	
• dynamic viscosity	0,39 mPa s at 20 °C
Explosive properties	Shall not be classified as explosive
Oxidising properties	none

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

9.2 Other information

Refractive index	1,344
Temperature class (EU, acc. to ATEX)	T1 (Maximum permissible surface temperature on the equipment: 450°C)

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

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.

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

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
EC50	3.560 mg/l	algae	ECHA	72 h
ErC50	9.696 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
LC50	>102 mg/l	fish	ECHA	7 d
LOEC	>102 mg/l	fish	ECHA	21 d
NOEC	102 mg/l	fish	ECHA	21 d

12.2 Process of degradability

The substance is readily biodegradable.

Theoretical Oxygen Demand with nitrification: 3,118 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.

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

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.

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.

SECTION 14: Transport information

14.1 UN number

1648

14.2 UN proper shipping name

ACETONITRILE

Hazardous ingredients

Acetonitrile

14.3 Transport hazard class(es)



Class

3 (flammable liquids)

14.4 Packing group

II (substance presenting medium danger)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

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



Special provisions (SP)	-
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 l


Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

EmS	F-E, S-D
Stowage category	B
• 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
	
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L

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)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**

Not listed.

- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

- **Restrictions according to REACH, Annex XVII**

Name of substance	CAS No	Wt%	Type of registration	No
Acetonitrile		100	1907/2006/EC annex XVII	3
Acetonitrile		100	1907/2006/EC annex XVII	40

- **List of substances subject to authorisation (REACH, Annex XIV)**

not listed

- **Seveso Directive**

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
P5c	flammable liquids (cat. 2, 3)	5.000	50.000	51)

Notation

51) Flammable liquids, categories 2 or 3 not covered by P5a and P5b

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

- **Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)**

VOC content 100 %

- **Directive on industrial emissions (VOCs, 2010/75/EU)**

VOC content 100 %

Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

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
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
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

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

SECTION 16: Other information

16.1 Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1	Remarks: For full text of Hazard- and EU Hazard-statements: see SECTION 16.		yes
2.2		Precautionary statements - prevention: change in the listing (table)	yes
8.1		Occupational exposure limit values (Workplace Exposure Limits): change in the listing (table)	yes
8.1		• human health values: change in the listing (table)	yes
8.1		• environmental values: change in the listing (table)	yes
14.3	Transport hazard class(es)	Transport hazard class(es): class 3 hazard - flammable liquids	yes
14.8	Particulars in the shipper's declaration: UN1648, ACETONITRILE, 3, II, 6°C c.c.	Particulars in the shipper's declaration: UN1648, ACETONITRILE, 3, II, 12,8°C c.c.	yes
14.8		Marine pollutant: -	yes
14.8		• International Civil Aviation Organization (ICAO-IATA/DGR)	yes
14.8		UN number: 1648	yes
14.8		Proper shipping name: Acetonitrile	yes
14.8		Particulars in the shipper's declaration: UN1648, Acetonitrile, 3, II	yes
14.8		Class: 3	yes
14.8		Packing group: II	yes
14.8		Danger label(s): 3	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Excepted quantities (EQ): E2	yes
14.8		Limited quantities (LQ): 1 L	yes

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
2017/2398/EU	Directive of the European Parliament and of the Council amending Directive 2004/37/EC on the protection of workers from the risks related to exposure to carcinogens or mutagens at work
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)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EH40/2005	EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-licence/)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
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
IOELV	indicative occupational exposure limit value
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
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
VOC	Volatile Organic Compounds
vPvB	very Persistent and very Bioaccumulative
WEL	workplace exposure limit

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Acetonitrile ROTISOLV® ≥99,98 %, Ultra LC-MS

article number: **HN40**

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)
- 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.