

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 06.01.2017

Version 22.1

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No.	100030
Product name	Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur
REACH Registration Number	01-2119471307-38-XXXX
CAS-No.	75-05-8

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

Identified uses	Reagent for analysis, Analytical and preparative chromatography In compliance with the conditions described in the annex to this safety data sheet.
-----------------	--

1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number **Please contact the regional company representation in your country.**

SECTION 2. Hazards identification**2.1 Classification of the substance or mixture****Classification (REGULATION (EC) No 1272/2008)**

Flammable liquid, Category 2, H225
Acute toxicity, Category 4, Oral, H302
Acute toxicity, Category 4, Inhalation, H332
Acute toxicity, Category 4, Dermal, H312
Eye irritation, Category 2, H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

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

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P240 Ground/bond container and receiving equipment.

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.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Index-No. 608-001-00-3

2.3 Other hazards

None known.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ CN	C ₂ H ₃ N (Hill)
Index-No.	608-001-00-3	
EC-No.	200-835-2	
Molar mass	41,05 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
---------	---------------------	----------------

Acetonitrile (<= 100 %)

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

75-05-8	01-2119471307-38-	
	XXXX	Flammable liquid, Category 2, H225 Acute toxicity, Category 4, H302 Acute toxicity, Category 4, H332 Acute toxicity, Category 4, H312 Eye irritation, Category 2, H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration.

Oxygen if necessary. Immediately call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, Nausea, Vomiting, Convulsions, Shortness of breath, Unconsciousness, respiratory arrest, cardiac arrest

May cause headache and dizziness.

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

Pay attention to flashback.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

nitrogen oxides, Hydrogen cyanide (hydrocyanic acid)

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Keep away from heat and sources of ignition. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Keep away from heat and sources of ignition. Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature see product label.

7.3 Specific end use(s)

See exposure scenario in the Annex to this MSDS.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

Derived No Effect Level (DNEL)

Worker DNEL, acute	Systemic effects	inhalation	68 mg/m ³
Worker DNEL, acute	Local effects	inhalation	68 mg/m ³
Worker DNEL, longterm	Systemic effects	dermal	32,2 mg/kg Body weight
Worker DNEL, longterm	Systemic effects	inhalation	68 mg/m ³
Worker DNEL, longterm	Local effects	inhalation	68 mg/m ³

Predicted No Effect Concentration (PNEC)

PNEC Fresh water	10 mg/l
PNEC Marine water	1 mg/l
PNEC Aquatic intermittent release	10 mg/l
PNEC Sewage treatment plant	32 mg/l
PNEC Soil	3,02 mg/kg
PNEC Fresh water sediment	45 mg/kg
PNEC Marine sediment	4,5 mg/kg

8.2 Exposure controls

Engineering measures

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	polychloroprene
Glove thickness:	0,65 mm
Break through time:	> 30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 720 Camapren® (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not empty into drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	ether-like
Odour Threshold	39,8 ppm
pH	No information available.
Melting point	-45,7 °C
Boiling point/boiling range	81,6 °C at 1.013 hPa
Flash point	2 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	3,0 %(V)
Upper explosion limit	17 %(V)

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Vapour pressure	97 hPa at 20 °C
Relative vapour density	1,42
Density	0,786 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	log Pow: -0,34 (IUCSID) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	Distillable in an undecomposed state at normal pressure.
Viscosity, dynamic	0,316 mPa.s at 25 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Ignition temperature	524 °C
----------------------	--------

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

10.2 Chemical stability

heat-sensitive

Distillable in an undecomposed state at normal pressure.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong bases, strong reducing agents

Risk of explosion with:

nitrates, perchlorates, perchloric acid

conc. sulfuric acid, with, Heat

Risk of ignition or formation of inflammable gases or vapours with:

Oxidizing agents, Nitric acid

nitrogen dioxide, with, Catalyst

Generates dangerous gases or fumes in contact with:

Acids

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, various plastics

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Mouse: 617 mg/kg

OECD Test Guideline 401

Symptoms: Nausea, Vomiting

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: No skin irritation

OECD Test Guideline 404

Eye irritation

Rabbit

Result: Eye irritation

OECD Test Guideline 405

Causes serious eye irritation.

Sensitisation

Buehler Test Guinea pig

Result: negative

Method: OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vivo

In vivo micronucleus test

Mouse

male and female

i.p.

Result: negative

Method: OECD Test Guideline 474

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

(External MSDS)

Mutagenicity (mammal cell test):

Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 476

Carcinogenicity

This information is not available.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

CMR effects

Carcinogenicity:

Based on available data the classification criteria are not met.

Mutagenicity:

Based on available data the classification criteria are not met.

Teratogenicity:

Based on available data the classification criteria are not met.

Reproductive toxicity:

Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

This information is not available.

11.2 Further information

After absorption:

Systemic effects:

Shortness of breath, Headache, Dizziness, Nausea, Convulsions, Unconsciousness, respiratory arrest, cardiac arrest

Symptoms may be delayed.

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

12.1 Toxicity

Toxicity to fish

semi-static test LC50 *Oryzias latipes* (Orange-red killifish): > 100 mg/l; 96 h
OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 *Daphnia magna* (Water flea): > 1.000 mg/l; 48 h
OECD Test Guideline 202

semi-static test NOEC *Daphnia magna* (Water flea): 960 mg/l; 21 d
OECD Test Guideline 202

Toxicity to algae

static test EC50 *Pseudokirchneriella subcapitata* (green algae): > 1.000 mg/l; 72 h
OECD Test Guideline 201

static test NOEC *Pseudokirchneriella subcapitata* (green algae): > 1.000 mg/l; 72 h
OECD Test Guideline 201

IC5 *Scenedesmus quadricauda* (Green algae): 7.300 mg/l; 8 d
(IUCLID) (maximum permissible toxic concentration)

Toxicity to bacteria

EC5 *Pseudomonas putida*: 680 mg/l; 16 h
(IUCLID) (maximum permissible toxic concentration)

12.2 Persistence and degradability

Biodegradability

70 %; 21 d
OECD Test Guideline 310
Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: -0,34

(IUCLID) Bioaccumulation is not expected.

Bioaccumulation

Bioconcentration factor (BCF): 0,3
Lepomis macrochirus (Bluegill sunfish)
Does not significantly accumulate in organisms.

Information taken from reference works and the literature.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

12.4 Mobility in soil

Distribution among environmental compartments

Adsorption/Soil

log Koc: 1,21

Mobile in soils (Lit.)

12.5 Results of PBT and vPvB assessment

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

12.6 Other adverse effects

Stability in water

DT50

> 9.999 d

at pH: 7

(calculated) Hydrolyses slowly.

Additional ecological information

Biological effects:

Hazard for drinking water supplies.

Discharge into the environment must be avoided.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 1648
14.2 Proper shipping name	ACETONITRILE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1648
14.2 Proper shipping name	ACETONITRILE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

14.1 UN number	UN 1648
14.2 Proper shipping name	ACETONITRILE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

14.6 Special precautions for user yes

EmS F-E S-D

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard SEVESO III
Legislation FLAMMABLE LIQUIDS
P5c
Quantity 1: 5.000 t
Quantity 2: 50.000 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of ≥ 0.1 % (w/w).

National legislation

Storage class 3

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

15.2 Chemical Safety Assessment

A Chemical Safety Assessment has been carried out according to regulation (EC) No. 1907/2006 (REACH) for this substance.

SECTION 16. Other information

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

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.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

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

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P240 Ground/bond container and receiving equipment.

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

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No.	100030
Product name	Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

lenses, if present and easy to do. Continue rinsing.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

EXPOSURE SCENARIO 1 (Industrial use)

1. Industrial use Reagent for analysis, Analytical and preparative chromatography)

Sectors of end-use

- SU 3* Industrial uses: Uses of substances as such or in preparations at industrial sites
SU 9 Manufacture of fine chemicals
SU 10 Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)

Chemical product category

- PC19* Intermediate
PC21 Laboratory chemicals

Process categories

- PROC1* Use in closed process, no likelihood of exposure
PROC2 Use in closed, continuous process with occasional controlled exposure
PROC3 Use in closed batch process (synthesis or formulation)
PROC4 Use in batch and other process (synthesis) where opportunity for exposure arises
PROC5 Mixing or blending in batch processes for formulation of preparations and articles (multistage and/ or significant contact)
PROC8a Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at non-dedicated facilities
PROC8b Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at dedicated facilities
PROC9 Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
PROC15 Use as laboratory reagent

Environmental Release Categories

- ERC1* Manufacture of substances
ERC2 Formulation of preparations
ERC4 Industrial use of processing aids in processes and products, not becoming part of articles
ERC6a Industrial use resulting in manufacture of another substance (use of intermediates)
ERC6b Industrial use of reactive processing aids
-

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling environmental exposure for: ERC1, SpERC ESVOC 1

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Amount used

Annual amount per site 8500 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 300
Emission or Release Factor: Air 0,5 %
Emission or Release Factor: Water 1 %
Emission or Release Factor: Soil 0,01 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Onsite sewage treatment plant
Flow rate of sewage treatment 2.000 m3/d
plant effluent
Sludge Treatment Sewage sludge should not be applied to natural soils.

2.2 Contributing scenario controlling environmental exposure for: ERC2

Amount used

Annual amount per site 5 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 20
Emission or Release Factor: Air 2,5 %
Emission or Release Factor: Water 2 %
Emission or Release Factor: Soil 0,01 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Municipal sewage treatment plant
Flow rate of sewage treatment 2.000 m3/d
plant effluent
Sludge Treatment Spreading as a worst case scenario

2.3 Contributing scenario controlling environmental exposure for: ERC4

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Amount used

Annual amount per site 500 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 200
Emission or Release Factor: Air 100 %
Emission or Release Factor: Water 100 %
Emission or Release Factor: Soil 5 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Municipal sewage treatment plant
Flow rate of sewage treatment 2.000 m3/d
plant effluent
Sludge Treatment Spreading as a worst case scenario
Remarks The concentration in the sewage treatment plant should be below the respective PNEC STP

2.4 Contributing scenario controlling environmental exposure for: ERC6a

Amount used

Annual amount per site 1000 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 100
Emission or Release Factor: Air 5 %
Emission or Release Factor: Water 2 %
Emission or Release Factor: Soil 0,10 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Municipal sewage treatment plant
Flow rate of sewage treatment 2.000 m3/d
plant effluent
Sludge Treatment Spreading as a worst case scenario

2.5 Contributing scenario controlling environmental exposure for: ERC6b

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Amount used

Annual amount per site 1000 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 100
Emission or Release Factor: Air 0,10 %
Emission or Release Factor: Water 5 %
Emission or Release Factor: Soil 0,025 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Municipal sewage treatment plant
Flow rate of sewage treatment 2.000 m3/d
plant effluent
Sludge Treatment Spreading as a worst case scenario

2.6 Contributing scenario controlling worker exposure for: PROC1, PROC2, PROC3, PROC4, PROC8b, PROC15

Product characteristics

Concentration of the Substance in Mixture/Article Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use) Medium volatile liquid
Process Temperature < 20 °C

Frequency and duration of use

Frequency of use 8 hours/day

Other operational conditions affecting workers exposure

Outdoor / Indoor Indoor without local exhaust ventilation (LEV)

Technical conditions and measures

Provide a good standard of general ventilation.

Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Wear suitable gloves tested to EN374.

Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice Use suitable eye protection. Wear suitable coveralls to prevent exposure to the skin.

2.7 Contributing scenario controlling worker exposure for: PROC5, PROC8a, PROC9

Product characteristics

Concentration of the Substance in Mixture/Article	Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use)	Medium volatile liquid
Process Temperature	< 20 °C

Frequency and duration of use

Frequency of use 8 hours/day

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor with local exhaust ventilation (LEV)
Remarks	Reduction factor for local exhaust ventilation (LEV) has not been used for the calculation of dermal exposure estimates.

Technical conditions and measures

Provide a good standard of general ventilation.

Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves tested to EN374.

Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice Use suitable eye protection. Wear suitable coveralls to prevent exposure to the skin.

3. Exposure estimation and reference to its source

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Environment

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	ERC1		Fresh water	0,175	EUSES
			Fresh water sediment	0,175	EUSES
			Marine water	0,175	EUSES
			Marine sediment	0,175	EUSES
			Soil	< 0,01	EUSES
			Sewage treatment plant	< 0,01	EUSES
2.2	ERC2		Fresh water	< 0,01	EUSES
			Fresh water sediment	< 0,01	EUSES
			Marine water	< 0,01	EUSES
			Marine sediment	< 0,01	EUSES
			Soil	< 0,01	EUSES
			Sewage treatment plant	< 0,01	EUSES
2.3	ERC4		Fresh water	0,32	EUSES
			Fresh water sediment	0,32	EUSES
			Marine water	0,32	EUSES
			Marine sediment	0,32	EUSES
			Soil	0,82	EUSES
			Sewage treatment plant	1	EUSES
2.4	ERC6a		Fresh water	0,12	EUSES
			Fresh water sediment	0,12	EUSES
			Marine water	0,12	EUSES
			Marine sediment	0,12	EUSES
			Soil	0,66	EUSES
			Sewage treatment plant	0,39	EUSES
2.5	ERC6b		Fresh water	0,30	EUSES
			Fresh water sediment	0,30	EUSES
			Marine water	0,30	EUSES
			Marine sediment	0,30	EUSES
			Soil	0,16	EUSES
			Sewage treatment plant	0,97	EUSES

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.6	PROC1	longterm, inhalative, systemic	< 0,01	ECETOC TRA 3
		longterm, dermal, systemic	< 0,01	ECETOC TRA 3
		longterm, combined, systemic	< 0,01	
2.6	PROC2	longterm, inhalative, systemic	0,13	ECETOC TRA 3
		longterm, dermal, systemic	< 0,01	ECETOC TRA 3
		longterm, combined, systemic	0,13	
2.6	PROC3	longterm, inhalative, systemic	0,25	ECETOC TRA 3
		longterm, dermal, systemic	< 0,01	ECETOC TRA 3
		longterm, combined, systemic	0,25	
2.6	PROC4	longterm, inhalative, systemic	0,50	ECETOC TRA 3
		longterm, dermal, systemic	0,04	ECETOC TRA 3
		longterm, combined, systemic	0,55	
2.6	PROC8b	longterm, inhalative, systemic	0,63	ECETOC TRA 3
		longterm, dermal, systemic	0,09	ECETOC TRA 3
		longterm, combined, systemic	0,71	
2.6	PROC15	longterm, inhalative, systemic	0,25	ECETOC TRA 3
		longterm, dermal, systemic	< 0,01	ECETOC TRA 3
		longterm, combined, systemic	0,25	
2.7	PROC5	longterm, inhalative, systemic	0,13	ECETOC TRA 3
		longterm, dermal, systemic	0,09	ECETOC TRA 3
		longterm, combined, systemic	0,21	
2.7	PROC8a	longterm, inhalative, systemic	0,13	ECETOC TRA 3
		longterm, dermal, systemic	0,09	ECETOC TRA 3
		longterm, combined, systemic	0,21	
2.7	PROC9	longterm, inhalative, systemic	0,13	ECETOC TRA 3
		longterm, dermal, systemic	0,04	ECETOC TRA 3
		longterm, combined, systemic	0,17	

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users;

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No.	100030
Product name	Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool SciDeEx® at www.merckmillipore.com/scideex.

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

EXPOSURE SCENARIO 2 (Professional use)

1. Professional use Reagent for analysis, Analytical and preparative chromatography)

Sectors of end-use

SU 22 Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Chemical product category

PC21 Laboratory chemicals

Process categories

PROC15 Use as laboratory reagent

Environmental Release Categories

ERC2 Formulation of preparations

ERC6a Industrial use resulting in manufacture of another substance (use of intermediates)

ERC6b Industrial use of reactive processing aids

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling environmental exposure for: ERC2

Amount used

Annual amount per site 5 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 20

Emission or Release Factor: Air 2,5 %

Emission or Release Factor: Water 2 %

Emission or Release Factor: Soil 0,01 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Municipal sewage treatment plant

Flow rate of sewage treatment plant effluent 2.000 m³/d

Sludge Treatment Spreading as a worst case scenario

2.2 Contributing scenario controlling environmental exposure for: ERC6a

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Amount used

Annual amount per site 1000 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 100
Emission or Release Factor: Air 5 %
Emission or Release Factor: Water 2 %
Emission or Release Factor: Soil 0,10 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Municipal sewage treatment plant
Flow rate of sewage treatment 2.000 m3/d
plant effluent
Sludge Treatment Spreading as a worst case scenario

2.3 Contributing scenario controlling environmental exposure for: ERC6b

Amount used

Annual amount per site 1000 t

Other given operational conditions affecting environmental exposure

Number of emission days per year 100
Emission or Release Factor: Air 0,10 %
Emission or Release Factor: Water 5 %
Emission or Release Factor: Soil 0,025 %

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant Municipal sewage treatment plant
Flow rate of sewage treatment 2.000 m3/d
plant effluent
Sludge Treatment Spreading as a worst case scenario

2.4 Contributing scenario controlling worker exposure for: PROC15

Product characteristics

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Concentration of the Substance in Mixture/Article	Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use)	Medium volatile liquid
Process Temperature	< 20 °C

Frequency and duration of use

Frequency of use 8 hours/day

Other operational conditions affecting workers exposure

Outdoor / Indoor Indoor without local exhaust ventilation (LEV)

Technical conditions and measures

Provide a good standard of general ventilation.

Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves tested to EN374.

Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice Use suitable eye protection. Wear suitable coveralls to prevent exposure to the skin.

3. Exposure estimation and reference to its source

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No. 100030
Product name Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Environment

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	ERC2		Fresh water	< 0,01	EUSES
			Fresh water sediment	< 0,01	EUSES
			Marine water	< 0,01	EUSES
			Marine sediment	< 0,01	EUSES
			Soil	< 0,01	EUSES
			Sewage treatment plant	< 0,01	EUSES
2.2	ERC6a		Fresh water	0,12	EUSES
			Fresh water sediment	0,12	EUSES
			Marine water	0,12	EUSES
			Marine sediment	0,12	EUSES
			Soil	0,66	EUSES
			Sewage treatment plant	0,39	EUSES
2.3	ERC6b		Fresh water	0,30	EUSES
			Fresh water sediment	0,30	EUSES
			Marine water	0,30	EUSES
			Marine sediment	0,30	EUSES
			Soil	0,16	EUSES
			Sewage treatment plant	0,97	EUSES

Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.4	PROC15	longterm, inhalative, systemic	0,25	ECETOC TRA 3
		longterm, dermal, systemic	< 0,01	ECETOC TRA 3
		longterm, combined, systemic	0,25	

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH

SAFETY DATA SHEET – Annex
according to Regulation (EC) No. 1907/2006

Catalogue No.	100030
Product name	Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC
Guidance Specific Environmental Release Categories (SPERCs).

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck
tool SciDeEx® at www.merckmillipore.com/scideex.