

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

1.1 Product identifiers

Product name : Acetonitrile InfinityLab gradient grade for LCMS

Catalogue No. : 5191-5101, 5191-5101-001

CAS-No. : 75-05-8

1.2 Other means of identification

No data available

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

Identified uses : Reagents and Standards for Analytical Chemical Laboratory Use.

1.4 Details of the supplier of the safety data sheet

Manufactured by : EMD Millipore Corporation
400 Summit Dr,
Burlington MA 01803 USA
An affiliate of Merck KGaA, Darmstadt, Germany.

Company : Agilent Technologies Australia Pty Ltd
679 Springvale Road
Mulgrave
Victoria 3170, Australia

Telephone : 1800 802 402

E-mail address : pdl-msds_author@agilent.com

1.5 Emergency telephone

Emergency Phone # : +61 290372994 (CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

Flammable liquids (Category 2), H225

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

Serious eye damage/eye irritation (Category 2A), H319

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

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H225

Highly flammable liquid and vapor.

H302 + H312 + H332
H319

Harmful if swallowed, in contact with skin or if inhaled.
Causes serious eye irritation.

Precautionary Statements

Prevention

P210

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

P233

Keep container tightly closed.

P261

Avoid breathing mist or vapors.

P264

Wash skin thoroughly after handling.

P280

Wear protective gloves/ eye protection/ face protection.

Response

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P312

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P337 + P313

If eye irritation persists: Get medical advice/ attention.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage

P403 + P235

Store in a well-ventilated place. Keep cool.

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

Formula : C₂H₃N
Molecular weight : 41.05 g/mol
CAS-No. : 75-05-8
EC-No. : 200-835-2
Index-No. : 608-001-00-3

Hazardous ingredients

Component	Classification	Concentration
Acetonitrile		
	Flam. Liq. 2; Acute Tox. 4; Eye Dam./Irrit. 2A; H225, H302, H332, H312, H319	<= 100 %

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

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

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

In case of eye contact

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

If swallowed

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

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures**5.1 Extinguishing media****Unsuitable extinguishing media**

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice 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.

5.4 Further information

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

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter 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. Chemisorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal 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.

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.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

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

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.3 no other specific uses are stipulated.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Acetonitrile	75-05-8	TWA	40 ppm 67 mg/m ³	Australia. Workplace Exposure Standards for Airborne Contaminants.
	Remarks	Skin absorption		
		STEL	60 ppm 101 mg/m ³	Australia. Workplace Exposure Standards for Airborne Contaminants.
		Skin absorption		

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Butoject® (KCL 898)

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Chloroprene
Minimum layer thickness: 0.65 mm
Break through time: 10 min
Material tested: KCL 720 Camapren®

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|--|
| a) Physical state | liquid |
| b) Color | colorless |
| c) Odor | ether-like |
| d) Melting point/freezing point | Melting point/range: -45.7 °C at 1,013 hPa |
| e) Initial boiling point and boiling range | 81.0 - 82.0 °C at 1,013.25 hPa |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 16 %(V)
Lower explosion limit: 4.4 %(V) |
| h) Flash point | 2.0 °C - closed cup |
| i) Autoignition temperature | No data available |
| j) Decomposition temperature | No data available |
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: 0.350 Pas at 20.00 °C |

- | | |
|--|--|
| m) Water solubility | 1,000 g/l at 25 °C completely soluble |
| n) Partition coefficient:
n-octanol/water | log Pow: -0.54 at 25 °C - Bioaccumulation is not expected. |
| o) Vapor pressure | 98.64 hPa at 20 °C |
| p) Density | 0.78 g/cm ³ at 20 °C |
| Relative density | No data available |
| q) Relative vapor
density | No data available |
| r) Particle
characteristics | No data available |
| | |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

- | | |
|---------------------------|----------------------|
| Surface tension | 29.0 mN/m at 20.0 °C |
| Relative vapor
density | 1.42 - (Air = 1.0) |

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

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

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Mouse - male and female - 617 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l - vapor

(OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1,500 mg/kg
(Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.
(OECD Test Guideline 405)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: US-EPA

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Result: Positive results were obtained in some in vitro tests.

Remarks: (National Toxicology Program)

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: Metabolic activation

Result: negative

Remarks: Sister chromatid exchange

Test system: *Saccharomyces cerevisiae*

Metabolic activation: without metabolic activation

Result: positive

Remarks: Cytogenetic analysis
(ECHA)

Test Type: In vitro mammalian cell gene mutation test
Test system: Mouse lymphoma test
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative

Test Type: Micronucleus test
Species: Mouse

Application Route: Intraperitoneal
Method: OECD Test Guideline 474
Result: negative

Carcinogenicity

No evidence of carcinogenicity in animal studies.

Reproductive toxicity

Animal testing did not show any effects on fertility.

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

No aspiration toxicity classification

11.2 Additional Information

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96 h Remarks: (ECHA)
Toxicity to algae	static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253) static test ErC50 - Phaeodactylum tricornutum - 9,696 mg/l - 72 h (ISO 10253)
Toxicity to bacteria	
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Oryzias latipes - 102 mg/l - 21 d (OECD Test Guideline 204)

12.2 Persistence and degradability

Biodegradability	Result: 70 % - Readily biodegradable. (OECD Test Guideline 310)
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12.3 Bioaccumulative potential

No bioaccumulation is to be expected ($\log Pow \leq 4$).

12.4 Mobility in soil

Not expected to adsorb on soil.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Biological effects:

Hazard for drinking water supplies.

Discharge into the environment must be avoided.

Avoid release to the environment.

Stability in water	DT50 - > 9,999 d pH 7 at 25 °C
	Remarks: (calculated)Hydrolyzes slowly.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. 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

14.1 UN number

ADR/RID: 1648	IMDG: 1648	IATA-DGR: 1648
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14.2 UN proper shipping name

ADR/RID:	ACETONITRILE
IMDG:	ACETONITRILE
IATA-DGR:	Acetonitrile

14.3 Transport hazard class(es)

ADR/RID: 3	IMDG: 3	IATA-DGR: 3
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14.4 Packaging group

ADR/RID: II	IMDG: II	IATA-DGR: II
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14.5 Environmental hazards

ADR/RID: no	IMDG Marine pollutant: no	IATA-DGR: no
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14.6 Special precautions for user

None

14.7 Incompatible materials

Other regulations

SECTION 15: Regulatory information**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

Therapeutic Goods (Poisons Standard)	:	No poison schedule number
Instrument		allocated

SECTION 16: Other information

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

H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H312	Harmful in contact with skin.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

Further information

The information contained in this document is based on Agilent's state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.