SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 06/12/2014 Version 1. 2

SECTION 1. Identification

Product identifier

Product number	100029
Product name	Acetonitrile hypergrade for LC-MS LiChrosolv®
Synonyms	ACN
CAS-No.	75-05-8

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

Identified uses	Reagent for analysis

Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821, United States of America | General Inquiries: +1-978-715-4321 | Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

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.

GHS-Labeling

Hazard pictograms



Signal Word
Danger

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

Precautionary Statements
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P240 Ground/bond container and receiving equipment.
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.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

OSHA Hazards
This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200). This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS and may deviate from the GHS information.

Other hazards
None known.

SECTION 3. Composition/information on ingredients

Formula	CH_3CN	C_2H_3N (Hill)
Synonyms	ACN	
Molar mass	41.05 g/mol	

Hazardous ingredients
Chemical Name (Concentration)
CAS-No.
acetonitrile (>= 90 % - <= 100 %)
75-05-8
Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures
Inhalation
After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

Skin contact
After skin contact: wash off with plenty of water. Remove contaminated clothing. Get medical attention.

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

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

Never give anything by mouth to an unconscious person.

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.

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

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.

Special hazards arising from the substance or mixture

Combustible.

Vapors 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 vapors possible in the event of fire.

Fire may cause evolution of:

nitrogen oxides, Hydrogen cyanide (hydrocyanic acid)

Advice for firefighters

Special protective equipment for fire-fighters

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/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

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, 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.

Environmental precautions

Do not empty into drains. Risk of explosion.

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.

SECTION 7. Handling and storage

Precautions for safe handling

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

Conditions for safe storage, including any incompatibilities

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

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
acetonitrile 75-05-8			
ACGIH	Time Weighted Average (TWA):	20 ppm	
	Skin designation:		Can be absorbed through the skin.
NIOSH/GUIDE	Recommended exposure limit (REL):	20 ppm 34 mg/m³	
OSHA_TRANS	PEL:	40 ppm 70 mg/m³	
Z1A	Time Weighted Average (TWA):	40 ppm 70 mg/m³	
	Short Term Exposure Limit (STEL):	60 ppm 105 mg/m³	

Engineering measures

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

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures
Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection
Safety glasses

Hand protection
Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:
Flame retardant antistatic protective clothing

Respiratory protection
required when vapors/aerosols are generated.
Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	ether-like
Odor Threshold	39.8 ppm
pH	No information available.
Melting point	-45.7 °C
Boiling point/boiling range	178.9 °F (81.6 °C) at 1,013 hPa
Flash point	36 °F (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)
Vapor pressure	97 hPa at 68 °F (20 °C)
Relative vapor density	1.42

Density	0.786 g/cm³ at 68 °F (20 °C)
Relative density	No information available.
Water solubility	at 68 °F (20 °C) soluble
Partition coefficient: n-octanol/water	log Pow: -0.34 (IUCLID) Bioaccumulation is not expected.
Autoignition temperature	No information available.
Decomposition temperature	Distillable in an undecomposed state at normal pressure.
Viscosity, dynamic	0.316 mPa.s at 77 °F (25 °C)
Explosive properties	Not classified as explosive.
Oxidizing properties	none
Ignition temperature	975 °F (524 °C)

SECTION 10. Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

heat-sensitive
Distillable in an undecomposed state at normal pressure.

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 vapors with:

Oxidizing agents, Nitric acid

nitrogen dioxide, with, Catalyst

Generates dangerous gases or fumes in contact with:

Acids

Conditions to avoid

Warming.

Incompatible materials
rubber, various plastics

Hazardous decomposition products
in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure
Inhalation, Eye contact, Skin contact

Target Organs
Respiratory system
cardiovascular system
Central nervous system
Liver
Kidneys

Acute oral toxicity
LD50 mouse: 617 mg/kg
OECD Test Guideline 401

absorption
Symptoms: Nausea, Vomiting

Acute inhalation toxicity
LC50 mouse: 6.022 mg/l; 4 h
OECD Test Guideline 403

absorption

Acute dermal toxicity
LD50 rabbit: > 2,000 mg/kg
OECD Test Guideline 402
(Regulation (EC) No 1272/2008, Annex VI)

absorption

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.

Sensitization
Buehler Test guinea pig
Result: negative
Method: OECD Test Guideline 406

Repeated dose toxicity
(External MSDS)

Genotoxicity in vivo
In vivo micronucleus test
mouse
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

CMR effects
Carcinogenicity:
Regarding the available data the classification criteria are not fulfilled.
Mutagenicity:
Regarding the available data the classification criteria are not fulfilled.
Teratogenicity:
Regarding the available data the classification criteria are not fulfilled.
Reproductive toxicity:
Regarding the available data the classification criteria are not fulfilled.

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

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

Aspiration hazard
Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or

equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

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)

Persistence and degradability

Biodegradability
70 %; 21 d
OECD Test Guideline 302B
Readily biodegradable.

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.)

Mobility in soil

Distribution among environmental compartments
Adsorption/Soil
log Koc: 1.21
Mobile in soils (Lit.)

Other adverse effects
Stability in water
DT50
> 9,999 d
at pH: 7
(calculated) Hydrolyzes slowly.

Additional ecological information
Biological effects:
Hazard for drinking water supplies.
Further information on ecology
Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number	UN 1648
Proper shipping name	ACETONITRILE
Class	3
Packing group	II
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 1648
Proper shipping name	ACETONITRILE
Class	3
Packing group	II
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

UN number	UN 1648
Proper shipping name	ACETONITRILE
Class	3
Packing group	II

Environmentally hazardous	--
Special precautions for user	yes
EmS	F-E S-D

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Flammable Liquid
Harmful if swallowed.
Eye irritant
Target organ effects
Harmful by skin absorption.
Harmful if inhaled.

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

SARA 311/312 Hazards

Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313

The following components are subject to reporting levels established by SARA Title III, Section 313:

Ingredients

acetonitrile	75-05-8	*100 %*

SARA 302

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

DEA List I

Not listed

DEA List II

Not listed

US State Regulations

Massachusetts Right To Know

Ingredients
acetonitrile

Pennsylvania Right To Know

Ingredients
acetonitrile

New Jersey Right To Know

Ingredients
acetonitrile

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA:	All components of the product are listed in the TSCA-inventory.
DSL:	All components of this product are on the Canadian DSL.

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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.

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.

Revision Date 06/12/2014

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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