



SIGMA-ALDRICH

Material Safety Data Sheet

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Section 1 - Product and Company Information

Product Name Acetonitrile, anhydrous, 99.8%
Product Number 271004
Brand Aldrich Chemical

Company Sigma-Aldrich
Address 3050 Spruce Street
City, State, Zip, Country SAINT LOUIS, MO 63103 US
Technical Phone: 800-325-5832
Fax: 800-325-5052
Emergency Phone: 314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313	EC no	Annex I Index Number
ACETONITRILE	75-05-8	Yes	200-835-2	608-001-00-3

Formula C₂H₃N
Synonyms Acetonitril (German, Dutch), Acetonitrile (ACGIH:OSHA), Cyanomethane, Cyanure de methyl (French), Ethanenitrile, Ethyl nitrile, Methanecarbonitrile, Methane, cyano-, Methylkyanid (Czech), NCI-C60822, RCRA waste number U003, USAF EK-488

Section 3 - Hazards Identification

Emergency Overview

Flammable (USA) Highly Flammable (EU). Harmful.
Harmful by inhalation, in contact with skin and if swallowed. Irritating to respiratory system and skin. Risk of serious damage to eyes. This material can produce a cyanide-like effect. Target organ(s): Central nervous system. Liver.

HMIS Rating
Health: 2* Flammability: 3 Reactivity: 0

NFPA Rating
Health: 2 Flammability: 3 Reactivity: 0

*additional chronic hazards present.

Section 4 - First Aid Measures

Oral Exposure

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

Inhalation Exposure

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

Dermal Exposure

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

Eye Exposure

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

Section 5 - Fire Fighting Measures

Flammable Hazards: Yes

Explosion Hazards

Vapor may travel considerable distance to source of ignition and flash back. Container explosion can occur under fire conditions. In advanced or massive fires the area should be evacuated and the fire should be fought from a remote explosion-resistant location.

Flash Point: 42 °F 6 °C

Explosion Limits: Lower: 4.4 % Upper: 16 %

Autoignition Temp: 274 °C **Flammability:** Yes

Extinguishing Media

Suitable

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

Firefighting

Protective Equipment

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

Specific Hazard(s)

Flammable liquid. Emits toxic fumes under fire conditions.

Specific Method(s) of Fire Fighting

For small (incipient) fire extinguishing, use a portable fire extinguisher rated for flammable liquid fires. For large fires, fixed fire suppression systems, such as a sprinkler system, should be capable of extinguishing a flammable liquid fire.

Section 6 - Accidental Release Measures

Procedure to be Followed in Case of Leak or Spill

Evacuate area. Shut off all sources of ignition.

Procedure(s) of Personal Precaution(s)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

Methods for Cleaning Up

Cover with dry-lime, sand, or soda ash. Place in covered containers using non-sparking tools and transport outdoors. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

Handling

User Exposure

Do not breathe vapor. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

Storage**Suitable**

Keep container closed. Keep away from heat, sparks, and open flame. Handle and store under nitrogen.

Special Requirements

Handle and store under inert gas.

Section 8 - Exposure Controls / PPE**Engineering Controls**

Safety shower and eye bath. Use nonsparking tools. Mechanical exhaust required.

Personal Protective Equipment**Respiratory**

Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator.

Hand

Compatible chemical-resistant gloves.

Eye

Chemical safety goggles.

General Hygiene Measures

Wash thoroughly after handling. Wash contaminated clothing before reuse.

Exposure Limits, RTECS

Country	Source	Type	Value
USA	ACGIH	STEL	60 PPM
USA	ACGIH	TWA	40 PPM
USA	MSHA Standard-air	TWA	40 PPM (70 MG/M3)
USA	OSHA.	PEL	8H TWA 40 PPM (70 MG/M3)
New Zealand	OEL		
Remarks: check ACGIH TLV			
USA	NIOSH	TWA	20 PPM

Section 9 - Physical/Chemical Properties

Appearance	Physical State	Color	Form	Odor
	Liquid	Colorless	Clear liquid	Pungent

Molecular Weight: 41.05 AMU

Property	Value	At Temperature or Pressure
pH	N/A	
BP/BP Range	81 - 82 °C	760 mmHg
MP/MP Range	-48 °C	
Freezing Point	N/A	
Vapor Pressure	72.8 mmHg	20 °C
Vapor Density	1.41 g/l	
Saturated Vapor Conc.	N/A	
SG/Density	0.786 g/cm3	
Bulk Density	N/A	
Odor Threshold	70 - 875 ppm	
Volatile%	N/A	
VOC Content	N/A	
Water Content	< 0.05 %	
Solvent Content	N/A	

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Evaporation Rate	5.79	
Viscosity	0.35 Pas	20 °C
Surface Tension	29.04 mN/m	20 °C
Partition Coefficient	Log Kow: -0.34	
Decomposition Temp.	N/A	
Flash Point °F	42 °F	
Flash Point °C	6 °C	

Method: closed cup
Method: closed cup

Explosion Limits	Lower: 4.4 % Upper: 16 %
Flammability	N/A
Autoignition Temp	274 °C
Refractive Index	1.344
Solubility	

Solubility in Water: soluble

Other Solvents: ETHYL ACETATE, ETHER, CHLOROFORM, C TETRACHLORIDE.

N/A = not available

Section 10 - Stability and Reactivity**Stability**

Stable

Stable.

Materials to Avoid

Acids, Bases, Oxidizing agents, Reducing agents, Alkali metals.

Hazardous Decomposition Products**Hazardous Decomposition Products**

Carbon monoxide, Carbon dioxide, Nitrogen oxides, Hydrogen cyanide.

Hazardous Polymerization**Hazardous Polymerization**

Will not occur.

Section 11 - Toxicological Information**Route of Exposure****Skin Contact**

May cause skin irritation.

Skin Absorption

Harmful if absorbed through skin.

Eye Contact

Causes severe eye irritation.

Inhalation

Harmful if inhaled. Material may be irritating to mucous membranes and upper respiratory tract.

Ingestion

Harmful if swallowed.

Target Organ(s) or System(s)

Central nervous system. Liver. Kidneys. Blood. Lungs.

Signs and Symptoms of Exposure

This material can produce a cyanide like effect. Always have a cyanide first-aid kit present when using this material. The onset of symptoms is generally delayed pending conversion to cyanide. Adverse effects may include nausea, vomiting, diarrhea, headache, dizziness, rashes and cyanosis. Other symptoms include mental excitement or depression, drowsiness, impaired perception, incoordination, stupor, coma, and death.

Conditions Aggravated by Exposure

Acetonitrile is metabolized in the liver to water, formic acid, and hydrogen cyanide. The cyanide is further metabolized to thiocyanate.

RTECS Number: AL7700000

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Toxicity Data

Oral - Rat: 2460 mg/kg (LD50)

Inhalation - Rat: 7,551 ppm (LC50)

Remarks: Behavioral: Altered sleep time (including change in righting reflex).
Behavioral: Convulsions or effect on seizure threshold.
Blood: Hemorrhage.

Intraperitoneal - Rat: 850 MG/KG (LD50)

Subcutaneous - Rat: 3500 MG/KG (LD50)

Intravenous - Rat: 1680 MG/KG (LD50)

Parenteral - Rat: 1100 MG/KG (LD50)

Oral - Mouse: 269 mg/kg (LD50)

Inhalation - Mouse: 2,693 ppm (LC50)

Remarks: Liver: Other changes.

Intraperitoneal - Mouse: 175 MG/KG (LD50)

Remarks: Sense Organs and Special Senses (Nose, Eye, Ear, and Taste): Eye: Corneal damage.
Behavioral: Ataxia.
Lungs, Thorax, or Respiration: Dyspnea.

Subcutaneous - Mouse: 4480 MG/KG (LD50)

Intravenous - Mouse: 612 MG/KG (LD50)

Oral - Cat: 200 mg/kg (LD50)

Inhalation - Cat: 18,000 mg/m³ (LC50)

Oral - Rabbit: 50 mg/kg (LD50)

Inhalation - Rabbit: 2,828 ppm (LC50)

Remarks: Behavioral: Altered sleep time (including change in righting reflex).
Behavioral: Convulsions or effect on seizure threshold.
Blood: Hemorrhage.

Skin - Rabbit: 1250 UL/KG (LD50)

Oral - Guinea pig: 177 mg/kg (LD50)

Inhalation - Guinea pig: 5,655 ppm (LC50)

Remarks: Behavioral: Altered sleep time (including change in righting reflex).
Behavioral: Convulsions or effect on seizure threshold.
Blood: Hemorrhage.

Oral - Mammal: 1670 mg/kg (LD50)

Irritation Data

Skin - Rabbit: 500 mg

Remarks: Mild irritation effect

Eyes - Rabbit: 20 mg

Remarks: Severe irritation effect

Skin - Rabbit: 500 mg

Remarks: Open irritation test

Chronic Exposure - Carcinogen

Result: This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

Rat - Inhalation: 400 PPM 6H/2Y 1

Result: Tumorigenic: Equivocal tumorigenic agent by RTECS criteria. Liver: Tumors.

NTP Carcinogen List

<u>Rating</u>	<u>Species</u>	<u>Route</u>
Equivocal evidence.	Rat	Inhalation
No evidence.	Mouse	Inhalation

ACGIH Carcinogen List

Rating
A4

Chronic Exposure - Teratogen

<u>Species</u>	<u>Dose</u>	<u>Route of Application</u>	<u>Exposure Time</u>
Hamster	300 MG/KG	Oral	(8D PREG)
Result: Specific Developmental Abnormalities: Musculoskeletal system.			
Hamster	8000 PPM/1H	Inhalation	(8D PREG)
Result: Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus). Specific Developmental Abnormalities: Musculoskeletal system.			

Chronic Exposure - Mutagen

<u>Species</u>	<u>Dose</u>	<u>Cell Type</u>	<u>Mutation test</u>
Hamster	5 GM/L	ovary	Sister chromatid exchange

Chronic Exposure - Reproductive Hazard

<u>Species</u>	<u>Dose</u>	<u>Route of Application</u>	<u>Exposure Time</u>
Rat	1800 PPM/6H	Inhalation	(6-20D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).			
Rabbit	390 MG/KG	Oral	(6-18D PREG)
Result: Maternal Effects: Other effects. Effects on Embryo or Fetus: Fetal death. Specific Developmental Abnormalities: Musculoskeletal system.			
Hamster	400 MG/KG	Oral	(8D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).			
Hamster	5000 PPM/1H	Inhalation	(8D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Specific Developmental Abnormalities: Central nervous system.			

Section 12 - Ecological Information

Acute Ecotoxicity Tests

Test Type

LC50 Fish

Species

Pimephales promelas (Fathead minnow)

Time:

Value:

96.0 h

1,640 mg/l

Test Type

EC50 Daphnia

Species

Daphnia magna

Time:

Value:

48.0 h

3,600 mg/l

Section 13 - Disposal Considerations

Appropriate Method of Disposal of Substance or Preparation

Contact a licensed professional waste disposal service to dispose of this material.
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable.
Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: Acetonitrile

UN#: 1648
Class: 3
Packing Group: Packing Group II
Hazard Label: Flammable liquid
PIH: Not PIH

IATA

Proper Shipping Name: Acetonitrile
IATA UN Number: 1648
Hazard Class: 3
Packing Group: II

Section 15 - Regulatory Information

EU Directives Classification

Symbol of Danger: F Xn

Indication of Danger

Highly Flammable. Harmful.

Risk Statements R: 11 20/21/22 36

Highly flammable. Harmful by inhalation, in contact with skin and if swallowed. Irritating to eyes.

Safety Statements S: 16 36/37

Keep away from sources of ignition - no smoking. Wear suitable protective clothing and gloves.

US Classification and Label Text

Indication of Danger

Flammable (USA) Highly Flammable (EU). Harmful.

Risk Statements

Harmful by inhalation, in contact with skin and if swallowed. Irritating to respiratory system and skin. Risk of serious damage to eyes.

Safety Statements

Keep away from sources of ignition - no smoking. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves, and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

US Statements

This material can produce a cyanide-like effect. Target organ(s): Central nervous system. Liver.

United States Regulatory Information

SARA Listed: Yes

Demimis: 1 %

Notes: This product is subject to SARA section 313 reporting requirements.

TSCA Inventory Item: Yes

Canada Regulatory Information

WHMIS Classification

This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.

DSL: Yes

NDSL: No

Section 16 - Other Information

Disclaimer

For R&D use only. Not for drug, household or other uses.

Warranty

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2007 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.