

MATERIAL SAFETY DATA SHEET

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Version 1.7

Section 1 - Product and Company Information

Product Name	ACETONITRILE, 99%
Product Number	110086
Brand	ALDRICH
Company	Sigma-Aldrich
Street Address	3050 Spruce Street
City, State, Zip, Country	SAINT LOUIS MO 63103 US
Technical Phone:	314 771 5765
Emergency Phone:	414 273 3850 Ext. 5996
Fax:	800 325 5052

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
ACETONITRILE	75-05-8	Yes
Formula	C2H3N	
Synonyms	Acetonitril (German, Dutch) * Acetonitrile (ACGIH:OSHA) * Cyanomethane * Cyanure de methyl (French) * Ethanenitrile * Ethyl nitrile * Methanecarbonitrile * Methane, cyano- * Methylcyanid (Czech) * NCI-C60822 * RCRA waste number U003 * USAF EK-488	
RTECS Number:	AL7700000	

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Flammable (USA) Highly Flammable (EU). Toxic (USA) Harmful (EU). Highly flammable. Harmful by inhalation and if swallowed. Toxic in contact with 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.

For additional information on toxicity, please refer to Section 11.

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

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

35.6 °F 2 °C Method: closed cup

EXPLOSION LIMITS

Lower: 4.4 % Upper: 16 %

AUTOIGNITION TEMP

523 °C

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: Carbon dioxide, dry chemical powder, or appropriate foam.

Unsuitable: Water may be effective for cooling, but may not effect extinguishment.

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.

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.

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	0.782 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	
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	35.6 °F 2 °C	Method: closed cup
Explosion Limits	Lower: 4.4 % Upper: 16 %	
Flammability	N/A	
Autoignition Temp	523 °C	
Refractive Index	1.344	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	Solubility in Water:soluble Other Solvents: MISCIBLE WITH METHANOL, ACETONE ETHYL ACETATE, ETHER C	

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.

TOXICITY DATA

Oral
Rat
2,460 mg/kg
LD50
Oral
Mouse
591 mg/kg
LD50
8 H
Inhalation
Rat
13,740 ppm
LC50
4 H
Inhalation
Mouse
3,587 ppm
LC50
Skin
Rabbit
> 2,000 mg/kg
LD50

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.

Species: Rat
Route of Application: Inhalation
Dose: 400 PPM
Exposure Time: 6H/2Y
Frequency: I
Result: Tumorigenic:Equivocal tumorigenic agent by RTECS criteria. Liver:Tumors.

NTP CARCINOGEN LIST

Rating: Equivocal evidence.
Species: Rat
Route: Inhalation

ACGIH CARCINOGEN LIST

Rating: A4

CHRONIC EXPOSURE - TERATOGEN

Species: Hamster
Dose: 300 MG/KG
Route of Application: Oral
Exposure Time: (8D PREG)

Result: Specific Developmental Abnormalities: Musculoskeletal system.

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

CHRONIC EXPOSURE - MUTAGEN

Species: Hamster
Dose: 5 GM/L
Cell Type: ovary
Mutation test: Sister chromatid exchange

CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Rat
Dose: 1800 PPM/6H
Route of Application: Inhalation
Exposure Time: (6-20D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Species: Rabbit
Dose: 390 MG/KG
Route of Application: Oral
Exposure Time: (6-18D PREG)
Result: Maternal Effects: Other effects. Effects on Embryo or Fetus: Fetal death. Specific Developmental Abnormalities: Musculoskeletal system.

Species: Hamster
Dose: 400 MG/KG
Route of Application: Oral
Exposure Time: (8D PREG)
Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

Species: Hamster
Dose: 5000 PPM/1H
Route of Application: Inhalation
Exposure Time: (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: 96 h
Value: 1,640 mg/l

Test Type: EC50 Daphnia
Species: Daphnia magna
Time: 48 h

Value: 3,600 mg/l

Test Type: LC50 Fish

Species: Pimephales promelas (Fathead minnow)

Time: 96 h

Value: 1,000 mg/l

Test Type: EC50 Daphnia

Species: Daphnia

Time: 24 h

Value: 10,000 mg/l

Test Type: IC50 Algae

Time: 72 h

Value: 7,300 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.

R: 11 20/21/22 36

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

S: 16 36/37

Safety Statements: 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).

Toxic (USA) Harmful (EU).

Risk Statements: Highly flammable. Harmful by inhalation and if swallowed. Toxic in contact with 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

DEMINIMIS: 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.
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