

SAFETY DATA SHEET



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ACETIC ACID IN ACETONITRILE AND WATER

SDS No. M0235

1. CHEMICAL PRODUCT

Product Name: Acetic Acid in Acetonitrile and Water

Synonyms:

Recommended Use: This product is recommended for laboratory and manufacturing use only. It is not recommended for drug, food or household use.

2. HAZARDS IDENTIFICATION



Classification:

Flammable Liquids: GHS Category 2

Skin Irritation: GHS Category 4

Eye Irritation: GHS Category 2

Specific Target Organ Toxicity for single exposure: GHS Category 3

Label Elements

Signal Word: DANGER!

Hazard Statements:

H225 – Highly flammable liquid and vapor.

H305 – May be harmful if swallowed and enters airways.

H319 – Causes serious eye irritation.

H332 – Harmful if inhaled.

Precautionary Statements:

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

P280 – Wear protective gloves/protective clothing/eye protection/face protection.

P303+P361+P353 – If on skin or hair: Remove/take off immediately all contaminated clothing. Rinse skin with water/shower.

P304+P312 - IF INHALED: Call a POISON CENTER or doctor/physician if you feel unwell.

P403 – Store in a well-ventilated place.

P501 – Dispose of contents/container at an approved waste disposal plant.

Emergency Overview

Highly flammable liquid and vapor. May be harmful if inhaled, absorbed through the skin, or swallowed. Affects the cardiovascular system, central nervous system, liver, and kidneys. May cause irritation to the eyes, skin, or respiratory tract. May metabolize to cyanide in the body. Target Organs: Kidneys, central nervous system, liver, respiratory system, cardiovascular system, eyes.

HMIS Rating:

Health – 2* Flammability – 3 Physical Hazard – 0 PPE – User supplied

NOTE: HMIS ratings use a numbering scale that ranges from 0 - 4 to indicate the degree of hazard. A value of zero means the chemical presents no hazard while a value of four indicates a high hazard. These ratings are based on the inherent properties of this chemical under expected conditions of normal use and are not intended to be used in emergency situations. PPE is determined by the user based on their needs and conditions.

3. COMPOSITION AND INFORMATION ON INGREDIENTS

| <u>Ingredient</u> | <u>CAS No</u> | <u>Percent</u> | <u>Hazardous</u> |
|-------------------|---------------|----------------|------------------|
| Acetonitrile | 75-05-8 | 54-56% | Yes |
| Water | 7732-18-5 | 44-46% | No |
| Acetic Acid | 64-19-7 | <1 | Yes |

4. FIRST-AID MEASURES

Inhalation: If inhaled, remove to fresh air. If breathing is labored or with coughing, give 100% supplemental oxygen. If not breathing, begin artificial respiration, but DO NOT give mouth-to-mouth resuscitation.

Ingestion: If swallowed, get medical attention immediately; DO NOT induce vomiting unless directed by medical personnel. Never give anything by mouth to an unconscious person. DO NOT give mouth-to-mouth resuscitation.

Skin Contact: Immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover irritated skin with an emollient or anti-bacterial cream. Soap and cold water may be used. Get medical attention immediately. Wash clothing before reuse. Thoroughly clean shoes before reuse.

Eye Contact: Check for and remove contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, lifting lower and upper eyelids occasionally. Get medical attention immediately.

Notes to Physician: Exposure should be treated as a cyanide poisoning. Effects may be delayed. For methemoglobinemia, administer oxygen alone or oxygen with Methylene Blue depending on the methemoglobin concentration in the blood. May be partially metabolized in the body. Always have a cyanide antidote kit on hand when working with cyanide compounds.

5. FIRE FIGHTING MEASURES

Flammability: Highly flammable liquid and vapor (GHS Category 2)

Auto-ignition Temperature: 534° C (975.2° F)

Flash Point: 2° C (35.6° F)

Flammable Limits: Lower Limit – 3.0 vol %, Upper Limit – 16.0 vol %

Products of Combustion: May decompose into toxic products under fire conditions (hydrogen cyanide, nitrogen oxides, carbon monoxide, carbon, dioxide).

Specific Fire Hazards: As in any fire, always wear self-contained breathing apparatus in pressure-demand (MSA/NIOSH approved or equivalent), and full protective gear. Use water spray to keep fire exposed containers cool. Approach fire from upwind to avoid hazardous vapors and toxic decomposition products. Vapors are heavier than air and may travel to a source of ignition and flash back. Vapors can spread along the ground and collect in low or confined areas.

Specific Explosion Hazards: None

Fire Fighting Media: Use water spray, dry chemical, carbon dioxide, or appropriate foam.

National Fire Protective Association: Health - 2, Flammability - 3, Reactivity - 0

NOTE: NFPA ratings use a numbering scale that ranges from 0 - 4 to indicate the degree of hazard. A value of zero means the chemical presents no hazard while a value of four indicates a high hazard. They are for use by emergency personnel to

address the hazards that are presented by short term, acute exposure to this product under fire, spill, or similar emergencies. Ratings involve data and interpretations that may vary from company to company.

6. ACCIDENTAL RELEASE MEASURES

Absorb spilled liquid with sorbent pads, socks, or other inert material such as vermiculite, sand, or earth. Provide ventilation to the affected area and remove all ignition sources. Approach the spill from upwind and pick up absorbed material and place it in a suitable container. Always use proper personal protective equipment as described in section 8.

7. HANDLING AND STORAGE

Precautions: Always use proper personal protective equipment as described in section 8. Wash thoroughly after handling. Ground and bond containers when transferring material. Avoid contact with eyes, skin, and clothing. Remove contaminated clothing and wash before reuse. Empty containers contain product residue (liquid and vapor) and can be dangerous. Keep container tightly closed and away from heat, spark, and flame. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks, or open flames. Use with adequate ventilation. Avoid breathing vapor or mist.

Storage: Keep in a flammables area away from all sources of ignition and oxidizing materials. Keep in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances. Protect from moisture.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Engineering Controls: Use explosion-proof ventilation equipment. Facilities storing or using the material should be equipped with eyewash station and a safety shower. Use adequate general or local exhaust ventilation to keep airborne concentrations below the permissible exposure limits.

Personal Protection: Wear chemical splash goggles. Use appropriate protective gloves and protective clothing to prevent skin exposure. A respiratory protection program that meets OSHA 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever possible. Always use a NIOSH or European Standard EN 149 approved respirator when necessary.

Exposure Limits (Acetonitrile):

ACGIH – 20 ppm TWA; Skin – potential significant contribution to overall exposure by cutaneous route

NIOSH – 20 ppm TWA; 34 mg/m³ TWA; 500 ppm IDLH

OSHA Final PELs – 40 ppm TWA; 70 mg/m³ TWA

Exposure Limits (Acetic Acid):

ACGIH – 10 ppm TWA; 15 ppm STEL

NIOSH – 10 ppm TWA; 25 mg/m³ TWA; 50 ppm IDLH

OSHA Final PELs – 10 ppm TWA; 25 mg/m³ TWA

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical State and Appearance: Clear, colorless liquid.

Odor: Sweetish, ethereal odor

Odor Threshold: 170 ppm

Molecular Formula: CH₃CN

Molecular Weight: 41.05

Auto-ignition Temperature: 534° C (975.2° F)

Flash Point: 2° C (35.6° F)

Flammable Limits: Lower Limit – 3.0 vol %, Upper Limit – 16.0 vol %

pH: Not available.

Boiling Point: 81.6° C @ 760 mm Hg

Freezing/Melting Point: -45° C

Decomposition Temperature: > 500° C

Specific Gravity: 0.7810 g/cm³

Vapor Density (Air=1): 1.42

Vapor Pressure: 88.8 mm Hg @ 25° C.

Viscosity: 0.36 cP 20° C

Solubility: Soluble

Conductivity (20°C): Conductive; Conductivity = 7×10^8 pS/m; Dielectric Constant = 37.5; Relaxation Time Constant = 5×10^{-7} seconds

10. STABILITY AND REACTIVITY

Stability: Stable under normal temperatures and pressures.

Conditions to Avoid: Ignition sources, excess heat, exposure to moist air or water.

Incompatibility With Various Substances: Strong oxidizing agents, strong reducing agents, strong acids.

Hazardous Decomposition Products: Hydrogen cyanide, nitrogen oxides, carbon monoxide, carbon dioxide.

Hazardous Polymerization: Will not occur.

11. TOXICOLOGICAL INFORMATION

Routes of Entry: Inhalation, skin absorption, skin contact

Acute Exposure:

INHALATION HAZARD - May be harmful if inhaled. Can irritate respiratory tract or possibly cause lung damage. Breaks down slowly in the body releasing cyanide ion and very high concentrations may produce cyanide poisoning. Symptoms are usually delayed several hours and include stomach or intestinal upset (nausea, vomiting, diarrhea) irritation (nose, throat, airways), headache, central nervous system depression (dizziness, drowsiness, weakness, fatigue, nausea, headache, unconsciousness), muscle weakness, kidney effects, effects on heart rate, loss of coordination, cyanosis (causes blue coloring of the skin and nails from lack of oxygen), lung edema (fluid buildup in the lung tissue). Victims may have an irregular heartbeat and feel tightness in the chest. Severe overexposure may result in death.

INGESTION HAZARD: May cause tissue anoxia with symptoms of dizziness, drowsiness, weakness, fatigue, nausea, headache, unconsciousness, effects on heart rate, loss of coordination, cyanosis (causes blue coloring of the skin and nails from lack of oxygen), and coma. Severe overexposure may result in death. In single dose toxicity studies by various routes, different animal species and different individuals of the same species displayed widely varying susceptibility to acetonitrile. The oral LD50 range for mammals was 140-6762 mg/kg body weight. A well conducted study of mice calculated an oral LD50 of 617 mg/kg.

SKIN CONTACT HAZARD: Causes mild irritation. May be absorbed into body. Absorbed material may be metabolized into cyanide which inhibits cytochrome oxidase impairing cellular respiration. Poisoning from dermal contact has been reported and an LD50 > 2000 mg/kg was obtained in a well conducted acute dermal toxicity study in rabbits.

EYE CONTACT HAZARD: Causes irritation and excessive tearing. May cause minor reversible damage.

Chronic Exposure: Acetonitrile is toxic to blood kidneys, liver, mucous membranes, gastrointestinal tract, upper respiratory tract, skin, eyes, and central nervous system. It may be toxic to the reproductive system. Repeated or prolonged exposure can produce target organ damage. Repeated exposure may produce general deterioration of health in target organs.

Acetonitrile may be metabolized to cyanide in the body which inhibits cytochrome oxidase impairing cellular respiration.

Classified as a toxin to the female reproductive system. Suspected of being a toxin to the male reproductive system.

Animal studies demonstrate that cyanide would cause toxic effects in the fetus at exposure levels that would be toxic to the parent.

Animal Toxicity:

Draize test, rabbit, eye: 100 uL/24H Moderate;

Inhalation, mouse: LC50 = 2693 ppm/1H;

Inhalation, rabbit: LC50 = 2828 ppm/4H;

Inhalation, rat: LC50 = 7551 ppm/8H;

Oral, mouse: LD50 = 269 mg/kg;

Oral, rabbit: LD50 = 50 mg/kg;

Oral, rat: LD50 = 2460 mg/kg;

Skin, rabbit: LD50 = 2000 mg/kg;

Carcinogenicity: Not listed as a carcinogen by ACGIH, IARC, NTP, or CA Prop 65

Epidemiology: Three volunteers were exposed for 4 hours at 40, 80, and 160 ppm acetonitrile. At 40 ppm, odor was detected, after which olfactory fatigue was noted. At this concentration, two persons had no signs of response, including no

appreciable blood or urinary cyanide or thiocyanate. The third person experienced slight tightness in the chest that evening. A sensation of cooling in the lungs was observed and persisted for 24 hours. Traces of urinary thiocyanate were recorded.

Teratogenicity: In most of the available assays, teratogenicity was associated with maternal toxicity. In a well conducted study, rats exposed by inhalation to acetonitrile did not result in significant fetal effects, even in concentrations that were overtly toxic to the dam. In this study, a maternal NOAEL of 1200 ppm and NOAEL of 1200 ppm with respect to developmental toxicity were established. A case-control study of pregnancy outcome among Finnish lab workers revealed no association between exposure to acetonitrile and increased risk of spontaneous abortion in mothers, or malformation and birth weight in their children.

Reproductive Effects: In relation to fertility, there is no information available in humans and there are no animal studies specifically investigating such effects. However, no changes were seen in weight of the right cauda or right testis and no effect on sperm motility in rats or mice exposed for 13 weeks with 100, 200, and 400 ppm to acetonitrile.

Mutagenicity: No information available.

Neurotoxicity: No information available.

12. ECOLOGICAL INFORMATION

Ecotoxicity:

Fish: Fathead minnow: 1150 ppm; 24 Hr; TLm (hard water);

Fish: Fathead minnow: 1000 mg/L; 96 Hr; TLm (soft water);

Fish: Bluegill/Sunfish: 1850 mg/L; 96 Hr; TLm (soft water);

Fish: Fathead minnow: 1640 mg/L; 96 Hr; LC50 (flow-bioassay);

Fish: Fathead minnow: 1640 mg/L; 96 Hr; EC50 (flow-bioassay) No data available;

Environmental Fate: Estimated Koc value = 16. Acetonitrile is expected to weakly adsorb to most soils based on the Koc value. Volatilization from soil surfaces and leaching into ground water is expected to be significant. Estimated BCF value = 0.3. This value indicates that acetonitrile will not significantly bioconcentrate in aquatic organisms or adsorb to suspended solids and sediments in water. Acetonitrile is unreactive towards photochemically-generated free radicals and direct photolysis in the gaseous phase. Biodegradable

13. DISPOSAL CONSIDERATIONS

Material that cannot be saved for recovery or recycling should be managed in an appropriate and approved waste facility. Processing, use, or contamination of this product may change the waste management options. Waste generators must decide if discarded material is a hazardous waste. State and local disposal regulations may differ from federal disposal definitions found in 40 CFR 261.3. Dispose of container and unused contents in accordance with federal, state and local requirements. This material is a "U" listed waste (U003 – ignitable, toxic waste).

14. TRANSPORT INFORMATION

US DOT

Proper Shipping Name: Acetonitrile solution

Hazard Class: 3

UN Number: UN1648

Packing Group: II

US IATA

Proper Shipping Name: Acetonitrile solution

Hazard Class: 3

UN Number: UN1648

Packing Group: II

US IMDG

Proper Shipping Name: Acetonitrile solution

Hazard Class: 3

UN Number: UN1648

Packing Group: II

15. REGULATORY INFORMATION

US Federal Regulations:

CERCLA Hazardous Substances: CAS#64-19-7 – 5000 lbs, 2270 kg final RQ; CAS# 75-05-8 – 5000 lbs final RQ; 2270 kg final RQ

SARA Section 302: Does not have a TPQ

SARA Codes: CAS# 64-19-7 – immediate, delayed, fire; CAS# 75-05-8 – immediate, delayed, fire;

Section 313: Acetonitrile (CAS# 75-05-8) is subject to SARA Title III Section 313 and 40 CFR 373 reporting requirements.

Clean Air Act: CAS# 75-05-8 is listed as a hazardous air pollutant (HAP).

Clean Water Act: CAS# 64-19-7 is listed as a Hazardous Substance.

OSHA: Not considered highly hazardous by OSHA.

US State Regulations:

CAS# 75-05-8 is on the following state right-to-know lists: California, New Jersey, Pennsylvania, and Massachusetts

Prop65: This product contains no chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Originally Prepared: 6/3/2015

Last Revised: 12/03/2020 – Updated pictograms.

The information contained herein is based on current knowledge and experience; no responsibility is accepted that the information is sufficient or correct in all cases. Users should consider these data only as a supplement to other information gathered by them and must make independent determinations of suitability and completeness of information from all sources to assure proper use and disposal of these materials and the safety and health of employees and customers and the protection of the environment.

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