

Chemical Safety Data Sheet MSDS / SDS

Adiponitrile SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: Adiponitrile

CAS: 111-69-3

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 3, Oral

Acute toxicity - Category 4, Inhalation

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H301 Toxic if swallowed

H332 Harmful if inhaled

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P330 Rinse mouth.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P317 Get medical help.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Adiponitrile
Common names and synonyms:	Adiponitrile
CAS number:	111-69-3
EC number:	203-896-3
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention. See Notes.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Give one or two glasses of water to drink. Refer for medical attention . See Notes.

Most important symptoms/effects, acute and delayed

This material is toxic by ingestion and inhalation. It produces disturbances of the respiration and circulation, irritation of the stomach and intestine, and loss of weight. It is irritating to skin and eyes. (EPA, 1998)

Indication of immediate medical attention and special treatment needed, if necessary

A person who has inhaled the vapors should be moved to an uncontaminated environment, and cardiopulmonary resuscitation should be administered. If the victim breathes with difficulty, oxygen should be given. In case of eye contact, flush with copious

water for at least 20 min and call a physician. In case of ingestion, induce vomiting and call a physician. For skin contact, wash with plenty of soap and water.

SECTION 5: Firefighting measures

Suitable extinguishing media

Use water spray, dry chemical, foam or carbon dioxide. use water spray to keep fire-exposed containers cool. approach fire from upwind to avoid hazardous vapors and toxic decomposition products.

Specific hazards arising from the chemical

Combustion products may contain hydrogen cyanide (hydrocyanic acid, HCN). Vapor may explode if ignited in an enclosed area. When heated to decomposition, it emits highly toxic fumes. Avoid oxidizing material. Hazardous polymerization may not occur. (EPA, 1998)

Special protective actions for fire-fighters

Use water spray, foam, powder, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: complete protective clothing including self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: complete protective clothing including self-contained breathing apparatus. Do NOT wash away into sewer. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Stop or control the leak, if this can be done without undue risk. Use water spray to cool and disperse vapors, and protect personnel. Approach release from upwind. Absorb in noncombustible material for proper disposal.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from strong oxidants, strong acids and food and feedstuffs. Ventilation along the floor. Separate from strong acids and oxidizing materials. Store in a cool, dry, well-ventilated location. Outside or detached storage is preferred.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 2 ppm as TWA; (skin)

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Slightly brown.
Odour:	Practically odorless.
Melting point/freezing point:	-5 - 6 °C.
Boiling point or initial boiling point and boiling range:	305.3 °C.
Flammability:	Class IIIA Combustible Liquid: Fl.P. at or above 140°F and below 200°F.
Lower and upper explosion limit/flammability limit:	LOWER 1.0% @ 200 DEG C
Flash point:	163 °C. Atm. press.:1 015 hPa.
Auto-ignition temperature:	475 °C. Atm. press.:1 019 hPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	9.1 cP @ 20 deg C; 2.6 cP @ 70 deg C
Solubility:	50 to 100 mg/mL at 73° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = -0.32. Temperature:25 °C.

Vapour pressure:	6.8 x10-4 mmHg. Temperature:25 °C.
Density and/or relative density:	0.968 g/ml. Temperature:20 °C.
Relative vapour density:	3.7 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on heating and on burning. This produces highly toxic hydrogen cyanide (see ICSC 0492). Reacts violently with strong oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

FLAMMABLE WHEN EXPOSED TO HEAT OR FLAME. ADIPONITRILE is incompatible with strong oxidizers. It is also incompatible with strong acids, strong bases and strong reducing agents. (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

Oxidizers (e.g., perchlorates, nitrates), strong acids (e.g., sulfuric acid) [Note: Decomposes above 194 degrees F, forming hydrogen cyanide].

Hazardous decomposition products

When heated to decomp releases vapors containing hydrocyanic acid.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 215 mg/kg. Remarks: 198-235 mg/kg (lower and upper limits).

Inhalation: LC50 - rat (male/female) - > 2.18 mg/L air (analytical).

Dermal: LD50 - rabbit (male) - 2 134 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: No human and no animal cancer data were available. Adiponitrile was negative for mutagenicity in Salmonella with and without activation. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: None.

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes and skin. Exposure could cause convulsions, unconsciousness and death. Medical observation is indicated.

STOT-repeated exposure

The substance may have effects on the blood and adrenals. This may result in anaemia and tissue lesions.

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 670 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: LC50 - *Daphnia magna* - > 1 000 mg/L - 72 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - > 97.4 mg/L - 72 h.

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Adiponitrile had a 5-day theoretical BOD of 40% in a river die-away study using unacclimated Ohio River water, 0.5-10 mg/l substrate concn and sewage inocula(1); a 12-day theoretical BOD was >100%(1); negligible degradation was observed after 2 days(1). At a substrate concn of 40 mg/l and 20 deg C, adiponitrile had theoretical CO₂ evolutions of 10 and 60% after 2 and 9 days, respectively, in river die-away studies using unacclimated Ohio River water and sewage inocula(1); at 5 deg C, theoretical CO₂ evolution was 10 and 60% after 7.5 and 33 days, respectively(1). At 20 deg C, effects of acclimation were examined by redosing at an initial substrate concn of 40 mg/l; the ratio of time it took to achieve 60% oxidation on 1st and 2nd feeding was 2.1 to 1(1). Adiponitrile was found to be toxic to one activated sludge unit after 72 hrs with a metal substrate concn of 500 mg/l; the other two sludge units had 2.2-2.8% theoretical BOD(2). Using a bench scale activated sludge unit, 93-98% BOD removal of adiponitrile was achieved using an influent concn equivalent to 275-350 mg/l BOD and a mean aeration retention time of 7-13 hours(3). Adiponitrile, present at 30 mg/l, reached 85% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 100 mg/l and the Japanese MITI test(4). Microorganisms (*Aeromonas* sp.) isolated from soil were able to use adiponitrile as their sole source of carbon(5).

Bioaccumulative potential

An estimated BCF of 3 was calculated for adiponitrile(SRC), using a log K_{ow} of -0.32(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of adiponitrile is estimated as 16(SRC), using a measured log Kow of -0.32(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that adiponitrile is expected to have very high mobility in soil(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2205 (For reference only, please check.)

IMDG: UN2205 (For reference only, please check.)

IATA: UN2205 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ADIPONITRILE (For reference only, please check.)

IMDG: ADIPONITRILE (For reference only, please check.)

IATA: ADIPONITRILE (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)
IMDG: III (For reference only, please check.)
IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No
IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Other Information

Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available. See ICSC 0492. The flash point of adiponitrile, technical grade is 93°C (o.c.). Do NOT take working clothes home.

Disclaimer: 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. We as supplier shall not be held liable for any