Chemical Safety Data Sheet MSDS / SDS

Benzonitrile SDS

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

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

Product identifier

Product name: Benzonitrile

CAS: 100-47-0

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

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 4, Oral
Acute toxicity - Category 4, Dermal

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Warning

Hazard statement(s)

H302 Harmful if swallowed
H312 Harmful in contact with skin

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

Response

P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P317 Get medical help.
P321 Specific treatment (see ... on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.

Storage

none

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:	Benzonitrile
Common names and synonyms:	Benzonitrile
CAS number:	100-47-0
EC number:	202-855-7
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.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. 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. Rest. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Benzonitrile may enter the human body by ingestion, absorption through the skin, or inhalation. The earliest symptoms of cyano compound intoxication may be weakness, headaches, confusion, and occasionally nausea and vomiting. The respiratory rate and depth will usually be increased at the beginning and at later stages become slow and gasping. Blood pressure is usually normal, especially in the mild or moderately severe cases, although the pulse rate is usually more rapid than normal. (USCG, 1999)

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial

respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Cyanide and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Foam, dry chemical, carbon dioxide. Water may be ineffective. Cool exposed containers with water. Wear goggles & self-contained breathing apparatus.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: Toxic hydrogen cyanide and oxides of nitrogen may form in fire. (USCG, 1999)

Special protective actions for fire-fighters

Use powder, AFFF, foam, 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: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Collect leaking liquid in sealable containers. 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

Remove all ignition sources. Ventilate area of spill or leak. Absorb liquids in vermiculite, dry sand, earth, or a similar material adn deposit in sealed containers. it maybe nessary to contain and dispose of this chemical as a hazardous waste.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Above 75°C use a closed system and ventilation. 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 food and feedstuffs. Well closed. Keep in a well-ventilated room.Conditions for safe storage, including any incompatibilities: Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Hygroscopic: Handle and store under inert gas.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

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 safety goggles or eye protection in combination with breathing protection.

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:	Colourless.
Odour:	Odor of volatile oil of almond
Melting point/freezing point:	-12.75 °C. Remarks:Melting Point.;-12.8 °C. Remarks:Freezing point.;-12.75°C. Remarks:Freezing point.
Boiling point or initial boiling point and boiling range:	190.7 °C. Remarks:No further details.
Flammability:	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	66 °C.
Auto-ignition temperature:	615 °C.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	kinematic viscosity (in mm2/s) = 1.054. Temperature:37.78°C.
Solubility:	1 to 5 mg/mL at 73° F (NTP, 1992)

Partition coefficient n-octanol/water:	log Pow = 1.5. Temperature:20 °C. Remarks:PH of the water phases and the saturated buffer solutions.;Pow = 35. Temperature:20 °C. Remarks:PH of the water phases and the saturated buffer solutions.
Vapour pressure:	Ca. 0.18 hPa. Temperature:Ca. 0 °C.;Ca. 0.38 hPa. Temperature:Ca. 10 °C.;Ca. 0.78 hPa. Temperature:Ca. 20 °C.
Density and/or relative density:	1.01 g/L.
Relative vapour density:	3.6 (NTP, 1992) (Relative to Air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on heating and on burning. This produces toxic fumes including hydrogen cyanide and nitrogen oxides. Reacts violently with strong acids. This produces highly toxic hydrogen cyanide. Attacks some plastics.

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

Combustible but burns with difficulty.The cyano group can be readily hydrolyzed in the presence of mineral acids to produce stable, moderately toxic benzoic acid . When heated to decomposition, it emits highly toxic fumes of nitrogen oxides and hydrogen cyanide [Sax, 9th ed., 1996, p. 353].

Conditions to avoid

no data available

Incompatible materials

Strong acids which can liberate hydrogen cyanide. Forms explosive mixture with air.

Hazardous decomposition products

When heated to decomp it emits toxic fumes of /cyanides and nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 1 000.

Inhalation: LC0 - rat (male/female) - 0.8 mg/L air.

Dermal: LD50 - rabbit (male/female) - 1 400 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

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the cellular respiration. This

may result in cyanosis. The effects may be delayed. Medical observation is indicated.

STOT-repeated exposure

no data available

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: TLm - Pimephales promelas - 116 mg/L - 24 h.

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water Flea) age < or =24 hr; Conditions: freshwater, static, 20-22 deg C, pH 7.6-7.7; Concentration: 200000 ug/L for 24 hr; Effect: intoxication, immobilization /formulation

Toxicity to algae: Scenedesmus quadricauda - 75 mg/L.

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Benzonitrile , present at 100 mg/L, reached 63.4% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(1). Other screening studies give similar results (63.4-80.8%) and benzonitrile is confirmed to be biodegradable according to the standard test of the Japanese Ministry of Industry and Trade (MITI) that employs a mixed inoculum obtained from freshwater, soil, and sludge(2-4). The theoretical oxygen demand (ThOD) for benzonitrile in Ohio River Water from Cincinnati and/or aged sewage sludge were 0, 60, 90% and/or 0, 40, 80% after 2, 5, and 12 days, respectively(5). The BOD for benzonitrile in a bench-scale activated sludge unit was measured to be 93-98%(6). The BOD for benzonitrile in river water, present at 50 ppm, was 7%(7). Benzonitrile achieved 100% degradation after 280 minutes in a phosphate buffer solution in the soil and after 500 minutes in a soil slurry(8). Benzonitrile also achieved 20% and 44% in ash and ash-amended soil slurries at 2000 minutes, respectively(8). Benzonitrile achieved 88% degradation after 8, 10, and 12.5 hours in char-amended soil, soil and washed-char-amended soil slurries(9).

Bioaccumulative potential

An estimated BCF of 5 was calculated in fish for benzonitrile(SRC), using a measured log Kow of 1.56(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 benzonitrile is estimated as 150(SRC), using a log Kow of 1.56(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that benzonitrile is expected to have moderate 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: UN2224 (For reference only, please check.)
IMDG: UN2224 (For reference only, please check.)
IATA: UN2224 (For reference only, please check.)

UN Proper Shipping Name

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