Chemical Safety Data Sheet MSDS / SDS

Phthalonitrile 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: Phthalonitrile

CAS: 91-15-6

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

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

uses:

Uses advised none

against:

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 3, Oral Acute toxicity - Category 3, Dermal Acute toxicity - Category 3, Inhalation Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

GHS label elements, including precautionary statements

Pictogram(s)

Signal word

Danger

Hazard statement(s)

H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled H412 Harmful to aquatic life with long lasting effects

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/...

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

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

P273 Avoid release to the environment.

Response

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

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

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P316 Get emergency medical help immediately.

P361+P364 Take off immediately all contaminated clothing and wash it before reuse.

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

Storage

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

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: Phthalonitrile

Common names and

Phthalonitrile

synonyms:

CAS number: 91-15-6

EC number: 202-044-8

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Rinse skin with plenty of water or shower.

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 a slurry of activated charcoal in water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

no data available

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

Minimum/Potential Fatal Human Dose

4(?). 4= very toxic: probable oral lethal dose (human) 50-500 mg/kg, between 1 teaspoon & 1 oz for 70 kg person (150 lb).

SECTION 5: Firefighting measures

Suitable extinguishing media

Use dry powder, carbon dioxide, foam.

Specific hazards arising from the chemical

Combustible. Gives off irritating or toxic fumes (or gases) in a fire. Finely dispersed particles form explosive mixtures in air.

Special protective actions for fire-fighters

Use dry powder, carbon dioxide, foam.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use

spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust. 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 and food and feedstuffs.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 1 mg/m3, as TWA

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.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state: YELLOW CRYSTALLINE POWDER WITH CHARACTERISTIC ODOUR.

Colour: NEEDLES FROM WATER OR PETROLEUM ETHER

Odour: Slightly aromatic

Melting -67°C(lit.)

point/freezing

point:

Boiling point or 115°C/50mmHg(lit.)

initial boiling point and boiling range:

Flammability: Combustible. Gives off irritating or toxic fumes (or gases) in a fire.

Lower and upper

no data available

explosion

limit/flammability

limit:

Flash point: 82°C(lit.)

Auto-ignition >580°C

temperature:

Decomposition no data available

temperature:

pH: no data available

Kinematic no data available

viscosity:

Solubility: Soluble in alcohol and ether

Partition $\log \text{Kow} = 0.99$

coefficient noctanol/water:

Vapour pressure: 0.05 millibar @ 20 deg C (3.75X10-2 mm Hg)

Density and/or 1.24

relative density:

Relative vapour no data available

density:

Particle no data available

characteristics:

SECTION 10: Stability and reactivity

Reactivity

Decomposes on heating. This produces toxic fumes including cyanide. On combustion, forms nitrogen oxides. Reacts with strong oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

No data. Decomposes on heating. This produces toxic fumes including cyanide. On combustion, forms nitrogen oxides. Reacts with strong oxidants.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of CN- and NOx /cyanides and nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Mouse oral 65 mg/kg

Inhalation: no data available

Dermal: no data available

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 may cause effects on the central nervous system.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful concentration of airborne particles can be reached quickly when dispersed.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

BCF values ranged from 0.8 to <5.5 for carp (Cyprinus carpio) exposed to 1,2-benzenedicarbonitrile (0.02 and 0.2 mg/l, respectively) for 6 weeks(1). According to a classification scheme(2), these BCF values suggest the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of 1,2-benzenedicarbonitrile is estimated as 82(SRC), using a measured log Kow of 0.99(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 1,2-benzenedicarbonitrile is expected to have 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: UN3439 (For reference only, please check.) IMDG: UN3439 (For reference only, please check.) IATA: UN3439 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: NITRILES, SOLID, TOXIC, N.O.S. (For reference only, please check.) IMDG: NITRILES, SOLID, TOXIC, N.O.S. (For reference only, please check.) IATA: NITRILES, SOLID, TOXIC, N.O.S. (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: I (For reference only, please check.)
IMDG: I (For reference only, please check.)
IATA: I (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

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Not 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/

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