Chemical Safety Data Sheet MSDS / SDS

Phenylacetonitrile 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: Phenylacetonitrile

CAS: 140-29-4

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

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H301 Toxic if swallowed H311 Toxic in contact with skin H330 Fatal if inhaled

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/...

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

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

P284 [In case of inadequate ventilation] wear respiratory protection.

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.

P320 Specific treatment is urgent (see ... on this label).

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: Phenylacetonitrile
Common names and Phenylacetonitrile

synonyms:

CAS number: 140-29-4
EC number: 205-410-5
Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

Poisonous. May be fatal if inhaled, swallowed, or absorbed through skin. Contact may cause burns to skin and eyes. (EPA, 1998)

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

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Keep unnecessary people away; isolate hazard area and deny entry. Stay upwind; keep out of low areas. Ventilate closed spaces before entering them. Wear positive pressure breathing apparatus and special protective clothing. Remove and isolate contaminated clothing at the site. Small fires: dry chemical, carbon dioxide, water spray, or foam. Large fires: water spray, fog, or foam. Move container from fire area if you can do it without risk. Fight fire from maximum distance. Dike fire control water for later disposal; do not scatter the material. (EPA, 1998)

Specific hazards arising from the chemical

When heated to decomposition, it emits very toxic fumes of cyanide and nitrogen oxides. Container may explode in heat of fire. Runoff from fire control water may give off poisonous gases. Avoid sodium hypochlorite. (EPA, 1998)

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

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

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Phenylacetoni	Phenylacetonitrile				
CAS No.	140-29-4	140-29-4				
	Limit value - E	Eight hours	Limit value - S	Limit value - Short term		
	ppm	_{mg/m} 3	ppm	_{mg/m} 3		
Latvia	?	0,8	?	?		
	Remarks					

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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state: Phenylacetonitrile, liquid is a colorless oily liquid with an aromatic odor. Insoluble in water

and slightly denser than water. Contact may irritate skin, eyes, and mucous membranes.

May be toxic by ingestion. Used to make other chemicals.

Colorless oily liquid Colour:

Odour: Aromatic odor

-24°C(lit.) Melting

point/freezing

point:

Boiling point or 230°C

initial boiling point and boiling range:

Flammability: no data available

Lower and upper explosion

no data available

limit/flammability

limit:

Flash point: 101°C(lit.)

Auto-ignition no data available

temperature:

Decomposition no data available

temperature:

pH: no data available

Kinematic no data available

viscosity:

Solubility: less than 1 mg/mL at 63° F (NTP, 1992)

Partition log Kow = 1.56

coefficient noctanol/water:

Vapour pressure: 0.1 mm Hg (20 °C)

Density and/or 1.01

relative density:

Relative vapour

density:

no data available

Particle no data available

characteristics:

SECTION 10: Stability and reactivity

Reactivity

This chemical is moisture sensitive. Insoluble in water.

Chemical stability

no data available

Possibility of hazardous reactions

PHENYLACETONITRILE can react with strong acids, strong bases, strong oxidizing agents and strong reducing agents. It may react vigorously with sodium hypochlorite. (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

Explosive reaction with sodium hypochlorite.

Hazardous decomposition products

When heated to decomposition it emits very toxic fumes of /hydrogen cyanide and nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Mouse oral 45.5 mg/kg

Inhalation: LC50 Mouse inhalation 0.05 mg/L/4hr

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

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

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

AEROBIC: Benzyl cyanide, present at 100 mg/L, reached 77% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L and the Japanese MITI test(1). This indicates rapid biodegradation is likely in the environment.

Bioaccumulative potential

An estimated BCF of 9 was calculated for benzyl cyanide(SRC), using a 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), provided the compound is not metabolized by the organism(SRP).

Mobility in soil

The Koc of benzyl cyanide is estimated as 170(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 benzyl cyanide is expected to have moderate mobility in soil.

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: UN2470 (For reference only, please check.) IMDG: UN2470 (For reference only, please check.) IATA: UN2470 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: PHENYLACETONITRILE, LIQUID (For reference only, please check.) IMDG: PHENYLACETONITRILE, LIQUID (For reference only, please check.) IATA: PHENYLACETONITRILE, LIQUID (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-stoffdatenbank/index-2.jsp

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

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