

Chemical Safety Data Sheet MSDS / SDS

3-PENTENENITRILE

Revision Date:2024-12-21 Revision Number:1

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

Product name : 3-PENTENENITRILE
CBnumber : CB0483061
CAS : 4635-87-4
EINECS Number : 225-060-7
Synonyms : 3-pent,3-pentenitrile

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
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

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

Flammable liquids, Category 3
Acute toxicity - Category 2, Oral
Acute toxicity - Category 3, Dermal
Acute toxicity - Category 2, Inhalation

Label elements**Pictogram(s)**

Signal word : Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H300 Fatal if swallowed
H311 Toxic in contact with skin
H330 Fatal if inhaled

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

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

P264 Wash ... thoroughly after handling.

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

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

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

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

P403+P235 Store in a well-ventilated place. Keep cool.

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-PENTENENITRILE
Synonyms	: 3-pent,3-pentenitrile
CAS	: 4635-87-4
EC number	: 225-060-7

MF : C5H7N
MW : 81.12

SECTION 4: First aid measures

Description of 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 and effects, both acute and delayed

Excerpt from ERG Guide 131 [Flammable Liquids - Toxic]: TOXIC; may be fatal if inhaled, ingested or absorbed through skin. Inhalation or contact with some of these materials will irritate or burn skin and eyes. Fire will produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

Indication of any immediate medical attention and special treatment needed

Rapid support of respiration and circulation is essential to successful treatment of cyanide intoxication. Massive cyanide overdoses have survived with only good supportive care. Immediate attention should be directed toward assisted ventilation, administration of 100% oxygen, insertion of intravenous lines, and institution of cardiac monitoring. Obtain an arterial blood gas immediately and correct any severe metabolic acidosis (pH below 7.15). Oxygen (100%) should be used routinely in moderate or severely symptomatic patients even in the presence of a normal pO₂, since 100% O₂ increases O₂ delivery, may reactivate cyanide-inhibited mitochondrial enzymes, and potentiates the effect of thiosulfate. Avoid mouth to mouth resuscitation during CPR in order to prevent self poisoning. Cyanides

SECTION 5: Firefighting measures

Extinguishing media

Excerpt from ERG Guide 131 [Flammable Liquids - Toxic]: CAUTION: All these products have a very low flash point: Use of water spray when fighting fire may be inefficient. SMALL FIRE: Dry chemical, CO₂, water spray or alcohol-resistant foam. LARGE FIRE: Water spray, fog or alcohol-resistant foam. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal; do not scatter the material. Use water spray or fog; do not use straight streams. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

Specific Hazards Arising from the Chemical

This chemical is combustible. (NTP, 1992)

Advice for firefighters

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

no data available

Biological limit values

no data available

Exposure 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

Eye/face protection

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

Skin protection

Wear fire/flammable 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

Information on basic physicochemical properties

Physical state	3-pentenitrile, [liquid] is a clear colorless to amber liquid. Less dense than water. Flash point 104°F. Boiling point 296°F. Generally stable and not liable to polymerization. May be toxic by skin absorption, inhalation or ingestion. Prolonged exposure may result in delayed cyanide poisoning. Avoid direct contact with vapors, mists or liquid. May produce cyanide gas and carbon monoxide during combustion. Used in the manufacture of various organic chemicals.
Colour	no data available
Odour	no data available
Melting point/freezing point	-3°C(lit.)
Boiling point or initial boiling point and boiling range	144°C(lit.)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	40°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	less than 1 mg/mL at 66° F (NTP, 1992)
Partition coefficient n-octanol/water	no data available
Vapour pressure	24.9 mm Hg (50 °C)
Density and/or relative density	0.827g/cm3
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

Nitriles, such as 3-PENTENENITRILE, may polymerize in the presence of metals and some metal compounds. They are incompatible with acids; mixing nitriles with strong oxidizing acids can lead to extremely violent reactions. Nitriles are generally incompatible with other oxidizing agents such as peroxides and epoxides. The combination of bases and nitriles can produce hydrogen cyanide. Nitriles are hydrolyzed in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids). These reactions generate heat. Peroxides convert nitriles to amides. Nitriles can react vigorously with reducing agents. Acetonitrile and propionitrile are soluble in water, but nitriles higher than propionitrile have low aqueous solubility. They are also insoluble in aqueous acids.

Conditions to avoid

no data available

Incompatible materials

Incompatible with strong oxidizers such as acids, acid salts, chlorates and nitrates. Cyanides

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- 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

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

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

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: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

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

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not 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?pagelD=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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