

Chemical Safety Data Sheet MSDS / SDS

3-PHENYLPROPIONITRILERevision Date:2025-02-01 Revision Number:1

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

Product name : 3-PHENYLPROPIONITRILE
CBnumber : CB1733015
CAS : 645-59-0
EINECS Number : 211-447-8
Synonyms : Benzenepropanenitrile,3-phenylpropanenitrile

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 : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

Precautionary statements

P264 Wash hands thoroughly after handling.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P321 Specific treatment (see ... on this label).
P405 Store locked up.

Hazard statementsH301 Toxic if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-PHENYLPROPIONITRILE
Synonyms	: Benzenepropanenitrile, 3-phenylpropanenitrile
CAS	: 645-59-0
EC number	: 211-447-8
MF	: C ₉ H ₉ N
MW	: 131.17

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO_x)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

□ SPEC.

□ HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Store in cool place. 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.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Splash contact Material: Chloroprene

Minimum layer thickness: 0,6 mm Break through time: 10 min

Material tested: Camapren? (KCL 722 / Aldrich Z677493, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our

customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	light yellow liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 2 °C - lit.
Initial boiling point and boiling range	113 °C at 10 hPa - lit.
Flash point	110 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,001 g/mL at 25 °C
Water solubility	1.68g/l (calculated)
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Mouse - 116 mg/kg

Inhalation: No data available Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: MW5604750

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Toxicity

No data available

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 3276 IMDG: 3276 IATA: 3276

UN proper shipping name

ADR/RID: NITRILES, LIQUID, TOXIC, N.O.S. (3-Phenylpropiononitrile) IMDG: NITRILES, LIQUID, TOXIC, N.O.S. (3-Phenylpropiononitrile) IATA: Nitriles, liquid, toxic, n.o.s. (3-Phenylpropiononitrile)

Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

SECTION 16: Other information

Abbreviations and acronyms

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

References

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

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

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

【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

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

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

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

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

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

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.