

Chemical Safety Data Sheet MSDS / SDS

2-Ethyl-2-phenylbutyronitrileRevision Date:2026-05-31 Revision Number:1

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

Product name : 2-Ethyl-2-phenylbutyronitrile
CBnumber : CB1233010
CAS : 5336-57-2
EINECS Number : 226-257-0
Synonyms : 2-Ethyl-2-phenylbutronitrile;2-ethyl-2-phenylbutanenitrile

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

P501 Dispose of contents/container to....
P405 Store locked up.
P330 Rinse mouth.
P321 Specific treatment (see ... on this label).
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P270 Do not eat, drink or smoke when using this product.
P264 Wash skin thoroughly after handling.

Hazard statementsH301 Toxic if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2-Ethyl-2-phenylbutyronitrile
Synonyms	: 2-Ethyl-2-phenylbutronitrile;2-ethyl-2-phenylbutanenitrile
CAS	: 5336-57-2
EC number	: 226-257-0
MF	: C12H15N
MW	: 173.25

SECTION 4: First aid measures

4.1 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.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid dust formation. Avoid breathing vapors, mist or gas.

Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

6.2 Environmental precautions

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

Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Hygiene measures

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

Storage class

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

7.3 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

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

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.

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 particle respirator type N99 (US) or type P2 (EN 143) 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.

Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	solid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	No data available
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	No data available
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available

l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	log Pow: 3,39
o) Vapor pressure	No data available
p) Density	No data available
Relative density	No data available
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available
Appearance	Light yellow to yellow Liquid

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - 100 mg/kg

Remarks: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 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.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH

Article 57(f) or Commission

Delegated regulation (EU) 2017/2100 or Commission

Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

Harmful to aquatic life.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 2811

IMDG: 2811

IATA: 2811

14.2 UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (2-ETHYL-2-PHENYLBUTYRONITRILE)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (2-ETHYL-2-PHENYLBUTYRONITRILE)

IATA: Toxic solid, organic, n.o.s. (2-ETHYL-2-PHENYLBUTYRONITRILE)

14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA: 6.1

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (E)

Further information : No data available

SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

International Chemical Weapons Convention : (CWC) Schedules of Toxic Chemicals and Precursors

Restrictions on the marketing and use of certain : dangerous substances and preparations

Regulation (EC) No 649/2012 of the European : Parliament and the Council concerning the export and import of dangerous chemicals

Candidate List of Substances of Very High : Concern for Authorisation National legislation

Seveso III: Directive 2012/18/EU of the H2 ACUTE TOXIC

European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR - Agreement concerning the International Carriage of Dangerous Goods by Road

AIIC - Australian Inventory of Industrial Chemicals

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

ECx - Concentration associated with x% response

ELx - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErCx - Concentration associated with x% growth rate response

GHS - Globally Harmonized System

GLP - Good Laboratory Practice
IARC - International Agency for Research on Cancer
IATA - International Air Transport Association
IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk
IC50 - Half maximal inhibitory concentration
ICAO - International Civil Aviation Organization
IECSC - Inventory of Existing Chemical Substances in China
IMDG - International Maritime Dangerous Goods
IMO - International Maritime Organization
ISHL - Industrial Safety and Health Law (Japan)
ISO - International Organisation for Standardization
KECI - Korea Existing Chemicals Inventory
LC50 - Lethal Concentration to 50 % of a test population
LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)
MARPOL - International Convention for the Prevention of Pollution from Ships
n.o.s. - Not Otherwise Specified
NO(A)EC - No Observed (Adverse) Effect Concentration
NO(A)EL - No Observed (Adverse) Effect Level
NOELR - No Observable Effect Loading Rate
NZIoC - New Zealand Inventory of Chemicals
OECD - Organization for Economic Co-operation and Development
OPPTS - Office of Chemical Safety and Pollution Prevention
PBT - Persistent, Bioaccumulative and Toxic substance
PICCS - Philippines Inventory of Chemicals and Chemical Substances
(Q)SAR - (Quantitative) Structure Activity Relationship
REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals
RID - Regulations concerning the International Carriage of Dangerous Goods by Rail
SADT - Self-Accelerating Decomposition Temperature
SDS - Safety Data Sheet
TCSI - Taiwan Chemical Substance Inventory
TECI - Thailand Existing Chemicals Inventory
TSCA - Toxic Substances Control Act (United States)
UN - United Nations
UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods
vPvB - Very Persistent and Very Bioaccumulative

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.