

Chemical Safety Data Sheet MSDS / SDS

3-PHENYLBUTYRIC ACID

Revision Date:2026-05-30 Revision Number:1

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

Product name : 3-PHENYLBUTYRIC ACID
CBnumber : CB4446275
CAS : 4593-90-2
EINECS Number : 224-987-4
Synonyms : 3-Phenylbutyric acid,3-phenylbutanoic acid

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

Warning

Precautionary statements

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

P264 Wash skin thoroughly after handling.

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

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

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

Hazard statements

H315 Causes skin irritation

H319 Causes serious eye irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-PHENYLBUTYRIC ACID
Synonyms	: 3-Phenylbutyric acid,3-phenylbutanoic acid
CAS	: 4593-90-2
EC number	: 224-987-4
MF	: C10H12O2
MW	: 164.2

SECTION 4: First aid measures

General advice

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

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting

Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products

Carbon oxides

Specific extinguishing methods

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7: Handling and storage

Handling

Avoidance of contact

Strong oxidizing agents Strong bases

Storage

Further information on storage conditions

Tightly closed. Dry.

Storage class

11, Combustible Solids

Recommended storage temperature

Recommended storage temperature see product label.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

No data available

Personal protective equipment

Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type

Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Eye/face protection

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

Safety glasses

Skin and body protection

protective clothing

Hand protection

Remarks

required

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

solid

Color

colorless

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

35 - 38 °C

Method: lit.

Boiling point/boiling range

170 - 172 °C (27 hPa)

Method: lit.

Flash point

110.00 °C

Method: closed cup

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

1.515 g/mL at 25 °C(lit.)

Density

1.515 g/mL (25 °C)

Method: lit.

Water solubility

9.254g/L(30 °C)

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

No data available

Oxidizing properties

No data available

Molecular weight

164.20 g/mol

Particle characteristics Particle size

No data available

Physical state

Solid

SECTION 10: Stability and reactivity

Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous

No data available reactions

Conditions to avoid

no information available

Incompatible materials

Strong oxidizing agents Strong bases

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: Causes skin irritation.

Serious eye damage/eye irritation

Remarks: Causes serious eye irritation.

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

May cause respiratory irritation.

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

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

SECTION 12: Ecological information

Ecotoxicity

Components:**3-Phenylbutyric acid:****Toxicity to fish**

Remarks: No data available

Persistence and degradability**Components:****3-Phenylbutyric acid:****Biodegradability**

Remarks: No data available

Bioaccumulative potential**Components:****3-Phenylbutyric acid:****Bioaccumulation**

Remarks: No data available

Mobility in soil**Components:****3-Phenylbutyric acid:****Stability in soil**

Remarks: No data available

Other adverse effects**Components:****3-Phenylbutyric acid:****Additional ecological information**

No data available

SECTION 13: Disposal considerations

Disposal methods**Waste from residues**

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

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Packing instruction (cargo aircraft) : Not applicable

Packing instruction (passenger aircraft) : Not applicable

IMDG-Code

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

EmS Code : Not applicable

Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation GB 6944/12268

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals

Not applicable

Hazardous Chemicals for Priority Management

Not applicable under SAWS

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not applicable

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number

B1A222214490

SECTION 16: Other information

Full text of other abbreviations

AIIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

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)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

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
Nch - Chilean Norm
NO(A)EC - No Observed (Adverse) Effect Concentration
NO(A)EL - No Observed (Adverse) Effect Level
NOELR - No Observable Effect Loading Rate
NOM - Official Mexican Norm
NTP - National Toxicology Program
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
SADT - Self-Accelerating Decomposition Temperature
SDS - Safety Data Sheet
TCSI - Taiwan Chemical Substance Inventory
TDG - Transportation of Dangerous Goods
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
WHMIS - Workplace Hazardous Materials Information System

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.