

## 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                                      |

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## 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

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## SECTION 5: Firefighting measures

### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) 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.

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## **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.

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## **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.

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## 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.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

solid

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#### 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

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## 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

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## 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.

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## 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

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## 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.

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## 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

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## **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<sub>x</sub> - Concentration associated with x% response

EL<sub>x</sub> - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC<sub>x</sub> - 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

IC<sub>50</sub> - 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.