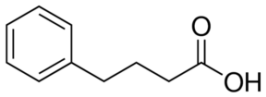
# 4-PHENYLBUTYRIC ACID EXTRA PURE

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878
Issue date: 3/20/2019 Revision date: 6/29/2026 Supersedes version of: 3/20/2019 Version: 1.0

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1. Product identifier

| | | |
|---|---|---|
| Product form | : | Substance |
| Trade name | : | 4-PHENYLBUTYRIC ACID EXTRA PURE |
| EC-No. | : | 217-341-8 |
| CAS-No. | : | 1821-12-1 |
| Product code | : | 5206C |
| Type of product | : | Carboxylic acids |
| Formula | : | C10H12O2 |
| Chemical structure | : |  |
| Synonyms | : | 4-Phenylbutanoic acid, Benzenebutanoic acid |

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

#### Relevant identified uses

| | | |
|---|---|---|
| Industrial/Professional use spec | : | Industrial<br>For professional use only |
| Use of the substance/mixture | : | Laboratory chemicals<br>Manufacture of substances |

### 1.3. Details of the supplier of the safety data sheet

LOBA CHEMIE PVT.LTD.
107 Wode House Road, Jehangir Villa, Colaba
400005 Mumbai
INDIA
T +91 22 6663 6663, F +91 22 6663 6699
info@lobachemie.com, www.lobachemie.com

### 1.4. Emergency telephone number

| | | |
|---|---|---|
| Emergency number | : | + 91 22 6663 6663 (9:00am - 6:00 pm) |

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

#### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Not classified

#### Adverse physicochemical, human health and environmental effects

To our knowledge, this product does not present any particular risk, provided it is handled in accordance with good occupational hygiene and safety practice.

### 2.2. Label elements

#### Labelling according to Regulation (EC) No. 1272/2008 [CLP]

No labelling applicable

### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

Substance type : Mono-constituent

| Name | Product identifier | % |
|---|---|---|
| 4-PHENYLBUTYRIC ACID | CAS-No.: 1821-12-1<br>EC-No.: 217-341-8 | 100 |

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general : If you feel unwell, seek medical advice.
First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing.
First-aid measures after skin contact : Wash skin with plenty of water.
First-aid measures after eye contact : Remove contact lenses, if present and easy to do. Continue rinsing. Rinse eyes with water as a precaution.
First-aid measures after ingestion : Rinse mouth. Call a poison center or a doctor if you feel unwell.
Self protection of the first-aider : Even though no specific hazards are defined, first-aiders should wear eye protection, gloves and disposable half mask. Consider additional protection if repeated or prolonged exposition is likely.

### 4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects after inhalation : None under normal conditions. Dust of the product, if present, may cause respiratory irritation after excessive inhalation exposure.
Symptoms/effects after skin contact : None under normal conditions. Dust may cause irritation in skin folds or by contact in combination with tight clothing.
Symptoms/effects after eye contact : None under normal conditions. Dust from this product may cause eye irritation.
Symptoms/effects after ingestion : None under normal conditions.

### 4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : dry chemical powder, alcohol-resistant foam, carbon dioxide (CO2). Water spray. Dry powder. Foam.
Unsuitable extinguishing media : Do not use a heavy water stream.

### 5.2. Special hazards arising from the substance or mixture

Fire hazard : No fire hazard.
Explosion hazard : No direct explosion hazard.
Hazardous decomposition products in case of fire : Toxic fumes may be released.

### 5.3. Advice for firefighters

Firefighting instructions : Fight fire from safe distance and protected location. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

General measures : Notify authorities if product enters sewers or public waters. Absorb spillage to prevent material damage.

#### For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.
Emergency procedures : Ventilate spillage area. Avoid contact with skin, eyes and clothing.

#### For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Use personal protective equipment as required. For further information refer to section 8: "Exposure controls/personal protection".
Emergency procedures : Evacuate unnecessary personnel.

### 6.2. Environmental precautions

Avoid release to the environment.

### 6.3. Methods and material for containment and cleaning up

For containment : Using a clean shovel, put the material in a dry container and cover without compressing it.
Methods for cleaning up : Mechanically recover the product. Clean contaminated surfaces with an excess of water.
Other information : Dispose of materials or solid residues at an authorized site.

### 6.4. Reference to other sections

For further information refer to section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Additional hazards when processed : Not expected to present a significant hazard under anticipated conditions of normal use.
Precautions for safe handling : Ensure good ventilation of the work station. Wear personal protective equipment. Avoid contact with skin and eyes.
Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Keep in a cool, well-ventilated place away from heat.
Storage conditions : Store in a well-ventilated place. Keep container tightly closed.
Packaging materials : Always store product in container of same material as original container.

### 7.3. Specific end use(s)

No additional information available

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No additional information available

### 8.2. Exposure controls

#### Appropriate engineering controls

**Appropriate engineering controls:**
Ensure good ventilation of the work station.

### Personal protection equipment

**Personal protective equipment:**
Wear recommended personal protective equipment.
**Personal protective equipment symbol(s):**



### Eye and face protection

**Eye protection:**
Chemical goggles or safety glasses

### Skin protection

**Skin and body protection:**
Wear a mask

**Hand protection:**
Protective gloves

### Respiratory protection

**Respiratory protection:**
Wear appropriate mask

### Environmental exposure controls

**Environmental exposure controls:**
Avoid release to the environment.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

| | | |
|---|---|---|
| Physical state | : | Solid |
| Colour | : | White to light yellow. White to beige. |
| Appearance | : | Crystalline powder or crystals. Chunks. Fused solid. |
| Molecular mass | : | 164.2 g/mol |
| Odour | : | Odourless. |
| Odour threshold | : | Not available |
| Melting point | : | 49 – 52 °C |
| Freezing point | : | Not applicable |
| Boiling point | : | 165 °C |
| Flammability | : | Non flammable |
| Lower explosion limit | : | Not applicable |
| Upper explosion limit | : | Not applicable |
| Flash point | : | > 113 °C |
| Auto-ignition temperature | : | Not applicable |
| Decomposition temperature | : | Not available |
| pH | : | Not available |
| pH solution | : | Not available |
| Viscosity, kinematic | : | Not applicable |
| Solubility | : | Water: Insoluble<br>Ethanol: Soluble |
| Partition coefficient n-octanol/water (Log Kow) | : | Not available |
| Partition coefficient n-octanol/water (Log Pow) | : | 2.42 |
| Vapour pressure | : | 0.000664 mm Hg |
| Vapour pressure at 50°C | : | Not available |
| Density | : | Not available |
| Relative density | : | Not available |
| Relative vapour density at 20°C | : | Not applicable |
| Particle size | : | Not available |

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

### 10.4. Conditions to avoid

Air contact. Direct sunlight. Moisture.

### 10.5. Incompatible materials

No additional information available

### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

## SECTION 11: Toxicological information

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

| | | |
|---|---|---|
| Acute toxicity (oral) | : | Not classified |
| Acute toxicity (dermal) | : | Not classified |
| Acute toxicity (inhalation) | : | Not classified |
| Skin corrosion/irritation | : | Not classified |
| Serious eye damage/irritation | : | Not classified |
| Respiratory or skin sensitisation | : | Not classified |
| Germ cell mutagenicity | : | Not classified |
| Carcinogenicity | : | Not classified |
| Reproductive toxicity | : | Not classified |
| STOT-single exposure | : | Not classified |
| STOT-repeated exposure | : | Not classified |
| Aspiration hazard | : | Not classified |

| 4-PHENYLBUTYRIC ACID EXTRA PURE (1821-12-1) | |
|---|---|
| Viscosity, kinematic | Not applicable |

### 11.2. Information on other hazards

No additional information available

## SECTION 12: Ecological information

### 12.1. Toxicity

| | | |
|---|---|---|
| Ecology - general | : | The product is not considered harmful to aquatic organisms nor to cause long-term adverse effects in the environment. |
| Hazardous to the aquatic environment, short–term (acute) | : | Not classified |

Hazardous to the aquatic environment, long–term (chronic) : Not classified

### 12.2. Persistence and degradability

| 4-PHENYLBUTYRIC ACID EXTRA PURE (1821-12-1) | |
|---|---|
| Persistence and degradability | Rapidly degradable |

### 12.3. Bioaccumulative potential

| 4-PHENYLBUTYRIC ACID EXTRA PURE (1821-12-1) | |
|---|---|
| Partition coefficient n-octanol/water (Log Pow) | 2.42 |

### 12.4. Mobility in soil

No additional information available

### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Endocrine disrupting properties

No additional information available

### 12.7. Other adverse effects

No additional information available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

Regional waste regulation : Disposal must be done according to official regulations.
Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.
Sewage disposal recommendations : Disposal must be done according to official regulations.
Product/Packaging disposal recommendations : Comply with applicable regulations for solid waste disposal. Disposal must be done according to official regulations.
Additional information : Do not re-use empty containers.
Ecological waste information : The waste of the product should be considered as hazardous as the product itself, with the likelihood of impacting the environment in the same way. Consider the handling and disposal of the waste as defined by the product itself.

## SECTION 14: Transport information

In accordance with ADR / IMDG / IATA / ADN / RID

### 14.1. UN number or ID number

Not regulated for transport

### 14.2. UN proper shipping name

Proper Shipping Name (ADR) : Not regulated
Proper Shipping Name (IMDG) : Not regulated
Proper Shipping Name (IATA) : Not regulated
Proper Shipping Name (ADN) : Not regulated
Proper Shipping Name (RID) : Not regulated

### 14.3. Transport hazard class(es)

**ADR**

Transport hazard class(es) (ADR) : Not regulated

**IMDG**
Transport hazard class(es) (IMDG) : Not regulated

**IATA**
Transport hazard class(es) (IATA) : Not regulated

**ADN**
Transport hazard class(es) (ADN) : Not regulated

**RID**
Transport hazard class(es) (RID) : Not regulated

### 14.4. Packing group

Packing group (ADR) : Not regulated
Packing group (IMDG) : Not regulated
Packing group (IATA) : Not regulated
Packing group (ADN) : Not regulated
Packing group (RID) : Not regulated

### 14.5. Environmental hazards

Other information : No supplementary information available

### 14.6. Special precautions for user

**Overland transport**
Not regulated

**Transport by sea**
Not regulated

**Air transport**
Not regulated

**Inland waterway transport**
Not regulated

**Rail transport**
Not regulated

### 14.7. Maritime transport in bulk according to IMO instruments

Not applicable

## SECTION 15: Regulatory information

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

**EU-Regulations**

**REACH Annex XVII (Restriction List)**

Not listed on REACH Annex XVII

**REACH Annex XIV (Authorisation List)**

Not listed on REACH Annex XIV (Authorisation List)

**REACH Candidate List (SVHC)**

Not listed on the REACH Candidate List

**PIC Regulation (Prior Informed Consent)**

Not listed on the PIC list (Regulation EU 649/2012)

**POP Regulation (Persistent Organic Pollutants)**

Not listed on the POP list (Regulation EU 2019/1021)

### Ozone Regulation (2024/590)

Not listed on the Ozone Depletion list (Regulation EU 2024/590)

### Council Regulation (EC) for the control of dual-use items

Not listed on the COUNCIL REGULATION (EC) of dual-use items.

### Explosives Precursors Regulation (EU 2019/1148)

Not listed on the Explosives Precursors list (EU)

### Drug Precursors Regulation (EC 273/2004)

Not listed on the Drug Precursors list (EU)

### National regulations

### Germany

| | | |
|---|---|---|
| Water hazard class (WGK) | : | WGK 3, Highly hazardous to water (Classification according to AwSV). |

### Netherlands

| | | |
|---|---|---|
| SZW List of Carcinogenic Substances | : | The substance is not listed |
| SZW List of Mutagenic Substances | : | The substance is not listed |
| SZW List of Reprotoxic Substances – Breastfeeding | : | The substance is not listed |
| SZW List of Reprotoxic Substances – Fertility | : | The substance is not listed |
| SZW List of Reprotoxic Substances – Development | : | The substance is not listed |

### Poland

| | | |
|---|---|---|
| Polish National Regulations | : | Act of 25 February 2011 on chemical substances and their mixtures (J. o L. No. 63, item 322 as amended; consolidated text J. o L. 2019, item 1225).<br>Act of 14 December 2012 on waste (J. o L. 2013, item 322 as amended; consolidated text J. o L. 2020, item 797).<br>The announcement of Marshal of the Sejm of the Republic of Poland dated 19 October 2016 concerning the consolidated text announcement of the decree on the management of packaging and packaging waste (J. o L. 2016, item 1863 as amended).<br>Decree of the Minister of Environment of 14 December 2014 on the catalogue of waste (J. o L. 2014, item 1923).<br>Act of 19 August 2011 on the Carriage of Dangerous Goods (J. o L. 2011 No. 227, item 1367 as amended; consolidated text J. o L. 2020, item 154).<br>Regulation of the Minister of Family, Labour and Social Policy of 12 June 2018 on the highest permissible concentration and intensity of noxious agents for health at work environment (J. o L. item 1286 as amended).<br>The announcement of Minister of Health dated 9 September 2016 concerning the consolidated text announcement of the decree of the Minister of Health of 30 December 2004 on health and safety at work related to exposure to chemical agents at work (J. o L. of 16 September 2016, item 1488)<br>Regulation of the Minister of Health of 2 February 2011 on tests and measurements of the noxious agents for health at work environment (J. o L. No. 33, item 166 as amended).<br>Regulation of the Minister of Environment of 9 December 2003 on particularly hazardous substances to the environment (J. o L. No. 217, item 2141).<br>ADR Agreement: Government Statement of 13 March 2023 on the entry into force of amendments to Annexes A and B to the Agreement concerning the International Carriage of Dangerous Goods by Road (ADR), signed in Geneva on 30 September 1957 (J. o. L. 2023, item 891)<br>Regulation of the Minister of Health of 25 August 2015 on the method of marking places, pipelines, and containers and tanks used for storing or containing hazardous substances or hazardous mixtures (J.o.L. 2015, item 1368 as amended) |

## 15.2. Chemical safety assessment

No chemical safety assessment has been carried out

## SECTION 16: Other information

| Abbreviations and acronyms: | |
|---|---|
| ACGIH | American Conference of Governmental Industrial Hygienists |
| ADN | European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways |
| ADR | European Agreement concerning the International Carriage of Dangerous Goods by Road |
| ATE | Acute Toxicity Estimate |
| BCF | Bioconcentration factor |
| BLV | Biological limit value |
| BOD | Biochemical oxygen demand (BOD) |
| CAS-No. | Chemical Abstracts Service number |
| CLP | Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008 |
| COD | Chemical oxygen demand (COD) |
| CSA | Chemical safety assessment |
| DMEL | Derived Minimal Effect level |
| DNEL | Derived-No Effect Level |
| EC-No. | European Community number |
| EC50 | Median effective concentration |
| ED | Endocrine disruptor |
| EN | European Standard |
| EWC | European waste catalogue |
| IARC | International Agency for Research on Cancer |
| IATA | International Air Transport Association |
| IMDG | International Maritime Dangerous Goods |
| LC50 | Median lethal concentration |
| LD50 | Median lethal dose |
| LOAEL | Lowest Observed Adverse Effect Level |
| Log Kow | Partition coefficient n-octanol/water (Log Kow) |
| Log Pow | Partition coefficient n-octanol/water (Log Pow) |
| MAK | maximum workplace concentration |
| NOAEC | No-Observed Adverse Effect Concentration |
| NOAEL | No-Observed Adverse Effect Level |
| NOEC | No-Observed Effect Concentration |
| N.O.S. | Not Otherwise Specified |
| OECD | Organisation for Economic Co-operation and Development |
| OEL | Occupational Exposure Limit |
| OSHA | Occupational Safety & Health Administration |
| PBT | Persistent Bioaccumulative Toxic |
| PNEC | Predicted No-Effect Concentration |
| PPE | Personal protection equipment |

| Abbreviations and acronyms: | |
|---|---|
| RID | Regulations concerning the International Carriage of Dangerous Goods by Rail |
| SDS | Safety Data Sheet |
| STP | Sewage treatment plant |
| TF | Technical function |
| ThOD | Theoretical oxygen demand (ThOD) |
| TLM | Median Tolerance Limit |
| TWA | Time Weighted Average |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and Very Bioaccumulative |
| UFI | Unique Formula Identifier |

Safety Data Sheet (SDS), EU

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.