

ALFAAA18115

4-Phenylbutyric acid

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: Product Description:	4-苯丁酸, 99% 4-Phenylbutyric acid
Cat No. :	A18115
Synonyms	Benzenebutanoic acid; Butanoic acid, 4-phenyl-
CAS No	1821-12-1
Molecular Formula	C10 H12 O2
Supplier	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
Emergency Telephone Number	For information US call: 001-800-227-6701 / Europe call: +32 14 57 52 11 Emergency Number US :001-201-796-7100 / Europe : +32 14 57 52 99 CHEMTREC Tel. No. US :001-800-424-9300 / Europe :001-703-527-3887
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use Uses advised against	Laboratory chemicals. No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State Powder Solid	Appearance Off-white	Odor Odorless
Emergency Overview The product contains no substances which at their given concentration are considered to be hazardous to health.		

Classification of the substance or mixture

Based on available data, the classification criteria are not met

Label Elements

None required

Physical and Chemical Hazards

None identified.

Health Hazards

The product contains no substances which at their given concentration are considered to be hazardous to health.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Benzenebutanoic acid	1821-12-1	99

SECTION 4. FIRST AID MEASURES**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

Inhalation

Remove from exposure, lie down. Remove to fresh air.

Ingestion

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. If possible drink milk afterwards.

Most important symptoms and effects

No information available.

Self-Protection of the First Aider

No special precautions required.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO₂). Dry chemical. Alcohol resistant foam.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Ensure adequate ventilation.

Environmental Precautions

See Section 12 for additional Ecological Information.

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Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Avoid contact with skin and eyes. Avoid contact with skin and clothing. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Avoid breathing vapors or mists. Do not ingest. If swallowed then seek immediate medical assistance. Wash thoroughly after handling.

Storage

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

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

Exposure Controls**Engineering Measures**

None under normal use conditions.

Personal protective equipment

Eye Protection	Wear safety glasses with side shields (or goggles) (European standard - EN 166)
Hand Protection	Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Butyl rubber				
Nitrile rubber				
Neoprene				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection	Long sleeved clothing
Respiratory Protection	No protective equipment is needed under normal use conditions.
Large scale/emergency use	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

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Recommended Filter type: Particle filter**Small scale/Laboratory use**

Maintain adequate ventilation

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141**Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls

No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Off-white	
Physical State	Powder Solid	
Odor	Odorless	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	49 - 52 °C / 120.2 - 125.6 °F	
Softening Point	No data available	
Boiling Point/Range	165 °C / 329 °F	@ 10 mmHg
Flash Point	> 110 °C / > 230 °F	Method - No information available
Evaporation Rate	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Vapor Pressure	No information available	
Vapor Density	Not applicable	Solid
Specific Gravity / Density	No data available	
Bulk Density	No data available	
Water Solubility	5.3 G/L WATER (40 DEGR. C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	Not applicable	Solid
Explosive Properties	No information available	
Oxidizing Properties	No information available	
Molecular Formula	C10 H12 O2	
Molecular Weight	164.2	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	No information available.
Hazardous Polymerization	No information available.
Conditions to Avoid	Incompatible products.
Materials to avoid	Strong oxidizing agents.

Hazardous Decomposition Products Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11. TOXICOLOGICAL INFORMATION

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Product Information	No acute toxicity information is available for this product
(a) acute toxicity;	
(b) skin corrosion/irritation;	No data available
(c) serious eye damage/irritation;	No data available
(d) respiratory or skin sensitization;	
Respiratory	No data available
Skin	No data available
(e) germ cell mutagenicity;	No data available
(f) carcinogenicity;	No data available
	There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	No data available
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	Not applicable
	Solid
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects,both acute and delayed	No information available

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
Persistence and Degradability	
Persistence	Soluble in water, Persistence is unlikely, based on information available.
Bioaccumulative Potential	Bioaccumulation is unlikely
Mobility in soil	The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility Highly mobile in soils
Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors

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**Persistent Organic Pollutant
Ozone Depletion Potential**

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS**Waste from Residues/Unused
Products**

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

Contaminated Packaging

Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used.

SECTION 14. TRANSPORT INFORMATION**Road and Rail Transport**

Not Regulated

IMDG/IMO

Not regulated

IATA

Not regulated

Special Precautions for User

No special precautions required

SECTION 15. REGULATORY INFORMATION**International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Benzenebutanoic acid	-	-	X	-	217-341-8	X	X	X	-		-	-

National Regulations**SECTION 16. OTHER INFORMATION****Prepared By**

Health, Safety and Environmental Department

Revision Date

22-Apr-2024

Revision Summary

New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Legend**CAS** - Chemical Abstracts Service**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances**PICCS** - Philippines Inventory of Chemicals and Chemical Substances**IECSC** - Chinese Inventory of Existing Chemical Substances**KECL** - Korean Existing and Evaluated Chemical Substances**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List**ENCS** - Japanese Existing and New Chemical Substances**AICS** - Australian Inventory of Chemical Substances**NZIoC** - New Zealand Inventory of Chemicals**WEL** - Workplace Exposure Limit**ACGIH** - American Conference of Governmental Industrial Hygienists**DNEL** - Derived No Effect Level**RPE** - Respiratory Protective Equipment**LC50** - Lethal Concentration 50%**NOEC** - No Observed Effect Concentration**PBT** - Persistent, Bioaccumulative, Toxic**TWA** - Time Weighted Average**IARC** - International Agency for Research on Cancer**PNEC** - Predicted No Effect Concentration**LD50** - Lethal Dose 50%**EC50** - Effective Concentration 50%**POW** - Partition coefficient Octanol:Water**vPvB** - very Persistent, very Bioaccumulative**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road**OECD** - Organisation for Economic Co-operation and Development**BCF** - Bioconcentration factor**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code**MARPOL** - International Convention for the Prevention of Pollution from Ships**ATE** - Acute Toxicity Estimate**VOC** - (Volatile Organic Compound)**Key literature references and sources for data**<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

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End of Safety Data Sheet