

ALFAAB23222

2-Phenylbutyric acid

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

产品说明: Product Description:	(+/-)-2-苯基丁酸, 98% 2-Phenylbutyric acid
Cat No. :	B23222
Synonyms	Benzeneacetic acid, alpha-ethyl.; alpha-phenyl butyric acid
CAS No	90-27-7
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	Laboratory chemicals.
Uses advised against	No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State Solid	Appearance Light yellow	Odor Odorless
Emergency Overview Harmful if swallowed.		

Classification of the substance or mixture

Acute Oral Toxicity	Category 4
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Label Elements



Signal Word

Warning

Hazard Statements

H302 - Harmful if swallowed

Precautionary Statements**Prevention**

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

Response

P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

Storage

P403 - Store in a well-ventilated place

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

None identified.

Health Hazards

Harmful if swallowed.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil.

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Benzeneacetic acid, .alpha.-ethyl-	90-27-7	98

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

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

Skin Contact

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

Inhalation

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

Ingestion

Clean mouth with water. Get medical attention.

Most important symptoms and effects

No information available.

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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.

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**

Ensure adequate ventilation, especially in confined areas. Ventilation systems. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

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 Butyl rubber Nitrile rubber Neoprene PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

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

Small scale/Laboratory use Maintain adequate ventilation

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	Light yellow	
Physical State	Solid	
Odor	Odorless	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	39 - 42 °C / 102.2 - 107.6 °F	
Softening Point	No data available	
Boiling Point/Range	270 - 272 °C / 518 - 521.6 °F	
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 data available	
Vapor Density	Not applicable	Solid
Specific Gravity / Density	No data available	
Bulk Density	No data available	
Water Solubility	Insoluble	
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	

SAFETY DATA SHEET

2-Phenylbutyric acid

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 (CO ₂).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(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

2-Phenylbutyric acid

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	Insoluble in water.
Bioaccumulative Potential	May have some potential to bioaccumulate
Mobility in soil	Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility
Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
Contaminated Packaging	Dispose of this container to hazardous or special waste collection point.
Other Information	Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

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
Benzeneacetic acid, .alpha.-ethyl-	-	-	X	X	201-982-5	X	-	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.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

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/NDSL - 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

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet