

MATERIAL SAFETY DATA SHEET

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Version 1.2

Section 1 - Product and Company Information

Product Name 2-PHENYLBUTYRIC ACID, 98%
Product Number P20955
Brand ALDRICH

Company Sigma-Aldrich Canada, Ltd
Street Address 2149 Winston Park Drive
City, State, Zip, Country Oakville ON L6H 6J8 CA
Technical Phone: 9058299500
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Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
(+/-)-2-PHENYLBUTYRIC ACID	90-27-7	No

Formula C10H12O2
Synonyms Benzeneacetic acid, alpha-ethyl- (9CI) *
alpha-Ethylphenylacetic acid * 2-Phenylbutanoic
acid * alpha-Phenyl butyric acid *
2-Phenylbutyric acid
RTECS Number: ET5957500

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Harmful.
Harmful if swallowed.

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE

In case of contact, immediately wash skin with soap and copious amounts of water.

EYE EXPOSURE

In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes.

Section 5 - Fire Fighting Measures

FLASH POINT

235 °F 113 °C Method: closed cup

AUTOIGNITION TEMP

N/A

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

EXPOSURE HAZARD(S)

Material: Harmful solid.

Section 6 - Accidental Release Measures

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Avoid inhalation. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep tightly closed. Store in a cool dry place.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Safety shower and eye bath. Mechanical exhaust required.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Government approved respirator.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash contaminated clothing before reuse. Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance

Color: Faintly beige
Form: Crystals

Property

Value

At Temperature or Pressure

Molecular Weight	164.2 AMU	
pH	N/A	
BP/BP Range	270 - 272 °C	760 mmHg
MP/MP Range	39 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	N/A	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	235 °F 113 °C	Method: closed cup
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	N/A	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Materials to Avoid: Strong oxidizing agents.

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.

Skin Absorption: May be harmful if absorbed through the skin.

Eye Contact: May cause eye irritation.

Inhalation: May be harmful if inhaled.

Ingestion: Harmful if swallowed.

SIGNS AND SYMPTOMS OF EXPOSURE

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

TOXICITY DATA

Oral

Mouse

1154 mg/kg

LD50

Intraperitoneal

Mouse

1320 MG/KG
LD50

Subcutaneous
Mouse
800 MG/KG
LD50

Intravenous
Mouse
320 MG/KG
LD50

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: None
Non-Hazardous for Transport: This substance is considered to be non-hazardous for transport.

IATA

Non-Hazardous for Air Transport: Non-hazardous for air transport.

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION

Symbol of Danger: Xn
Indication of Danger: Harmful.
R: 22
Risk Statements: Harmful if swallowed.
S: 22 36
Safety Statements: Do not breathe dust. Wear suitable protective clothing.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Harmful.
Risk Statements: Harmful if swallowed.
Safety Statements: Wear suitable protective clothing.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: No
TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: No
NDSL: Yes

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. Copyright 2005 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.