

Revision Date 05-Mar-2019

Revision Number 2

**SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING**

**1.1. Product identification**

**Product Description:** (R)-(-)-2-Phenylbutyric acid  
**Cat No. :** 378520000; 378520010; 378520050  
**CAS-No** 938-79-4  
**Molecular Formula** C10 H12 O2

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

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

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

**Company** **UK entity/business name**  
 Fisher Scientific UK  
 Bishop Meadow Road, Loughborough,  
 Leicestershire LE11 5RG, United Kingdom

**EU entity/business name**  
 Acros Organics BVBA  
 Janssen Pharmaceuticaaan 3a  
 2440 Geel, Belgium

**E-mail address** begel.sdsdesk@thermofisher.com

**1.4. Emergency telephone number**

For information **US** call: 001-800-ACROS-01 / **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

**SECTION 2: HAZARDS IDENTIFICATION**

**2.1. Classification of the substance or mixture**

**CLP Classification - Regulation (EC) No 1272/2008**

**Physical hazards**

Based on available data, the classification criteria are not met

**Health hazards**

Acute oral toxicity	Category 4 (H302)
Skin Corrosion/irritation	Category 2 (H315)
Serious Eye Damage/Eye Irritation	Category 2 (H319)
Specific target organ toxicity - (single exposure)	Category 3 (H335)

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

## Environmental hazards

Based on available data, the classification criteria are not met

## 2.2. Label elements



Signal Word

Warning

## Hazard Statements

- H315 - Causes skin irritation
- H302 - Harmful if swallowed
- H319 - Causes serious eye irritation
- H335 - May cause respiratory irritation

## Precautionary Statements

- P261 - Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray
- P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell
- P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
- P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection
- P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

## 2.3. Other hazards

No information available

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008
Benzeneacetic acid, .alpha.-ethyl-, (R)-	938-79-4		100	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302)

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

ACR37852

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Obtain medical attention.
<b>Ingestion</b>	Clean mouth with water. Get medical attention.
<b>Inhalation</b>	Remove from exposure, lie down. Move to fresh air. If not breathing, give artificial respiration. Obtain medical attention.
<b>Self-Protection of the First Aider</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

No information available.

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

**Notes to Physician** Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

#### 5.1. Extinguishing media

##### **Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam.

##### **Extinguishing media which must not be used for safety reasons**

No information available.

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

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

##### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

#### 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

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

Ensure adequate ventilation.

#### 6.2. Environmental precautions

See Section 12 for additional ecological information.

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

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal.

## 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Avoid contact with skin and eyes. Do not breathe vapors or spray mist.

#### Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing before re-use. Wash hands before breaks and at the end of workday.

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

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

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### 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.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

**Derived No Effect Level (DNEL)** No information available

<u>Route of exposure</u>	<b>Acute effects (local)</b>	<b>Acute effects (systemic)</b>	<b>Chronic effects (local)</b>	<b>Chronic effects (systemic)</b>
Oral Dermal Inhalation				

**Predicted No Effect Concentration (PNEC)** No information available.

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

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** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

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

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure

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.

**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

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

<b>Appearance</b>	Colorless	
<b>Physical State</b>	Viscous liquid	Liquid
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	130 °C / 266 °F	@ 3 mbar
<b>Flash Point</b>	110 °C / 230 °F	<b>Method</b> - No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

Vapor Pressure	No data available	
Vapor Density	No data available	(Air = 1.0)
Specific Gravity / Density	1.055	
Bulk Density	Not applicable	Liquid
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	No data available	
Explosive Properties	No information available	
Oxidizing Properties	No information available	

## 9.2. Other information

Molecular Formula	C10 H12 O2
Molecular Weight	164.2

## SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Stable.

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.  
Hazardous Reactions No information available.

10.4. Conditions to avoid Incompatible products.

10.5. Incompatible materials Strong oxidizing agents.

10.6. Hazardous decomposition products Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on toxicological effects

#### Product Information

(a) acute toxicity;  
Oral Category 4  
Dermal No data available  
Inhalation No data available

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

**(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;** Category 3  
**Results / Target organs** Respiratory system.

**(i) STOT-repeated exposure;** No data available  
**Target Organs** None known.

**(j) aspiration hazard;** No data available

**Other Adverse Effects** The toxicological properties have not been fully investigated.

**Symptoms / effects,both acute and delayed** No information available

## SECTION 12: ECOLOGICAL INFORMATION

**12.1. Toxicity**

**Ecotoxicity effects** Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

**12.2. Persistence and degradability**

**Persistence** Insoluble in water, Persistence is unlikely, based on information available.

**12.3. Bioaccumulative potential** May have some potential to bioaccumulate

**12.4. Mobility in soil**

Spillage unlikely to penetrate soil The product is insoluble and sinks in water The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility.

**12.5. Results of PBT and vPvB assessment**

No data available for assessment.

**12.6. Other adverse effects**

**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

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

#### 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.

#### European Waste Catalogue (EWC)

According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.

#### 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

### IMDG/IMO

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

### ADR

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

### IATA

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

#### 14.5. Environmental hazards

No hazards identified

#### 14.6. Special precautions for user

No special precautions required

#### 14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

X = listed.

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	IECSC	AICS	KECL
Benzeneacetic acid, .alpha.-ethyl-, (R)-	-	-		-	-	-	-	X	-	-	-



# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

## National Regulations

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment.

### 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

### 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

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - Volatile Organic Compounds

### Key literature references and sources for data

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

### 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.

Revision Date

05-Mar-2019

Revision Summary

Not applicable.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006**

### 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

# SAFETY DATA SHEET

(R)-(-)-2-Phenylbutyric acid

Revision Date 05-Mar-2019

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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**