



# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

## SECTION 1: Identification

### 1.1 GHS Product identifier

**Product name** 3-phenyl-L-alanine

### 1.2 Other means of identification

**Product number** -

**Other names** Benzenepropanethioic acid,S-phenyl ester;  
Thiohydrozimtsaeurephenylester; L-Phenylalanine

### 1.3 Recommended use of the chemical and restrictions on use

**Identified uses** Industrial and scientific research use.

**Uses advised against** no data available

### 1.4 Supplier's details

**Company** Shanghai Yien Chemical Technology Co., Ltd  
**Address** Building 6, 28 Yingong Road, Fengxian District, Shanghai  
Chemical Industry Zone, Shanghai, 201400, China  
**Telephone** +86-400-133-2688

### 1.5 Emergency phone number

**Emergency phone number** +86-400-133-2688

**Service hours** Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

## SECTION 2: Hazard identification

### 2.1 Classification of the substance or mixture

Not classified.

### 2.2 GHS label elements, including precautionary statements

**Pictogram(s)** No symbol.  
**Signal word** No signal word  
**Hazard statement(s)** none  
**Precautionary statement(s)**  
**Prevention** none  
**Response** none  
**Storage** none  
**Disposal** none

### 2.3 Other hazards which do not result in classification

no data available

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
3-phenyl-L-alanine	3-phenyl-L-alanine	63-91-2	200-568-1	100%

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## SECTION 4: First-aid measures

### 4.1 Description of necessary first-aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

### 4.2 Most important symptoms/effects, acute and delayed

ACUTE/CHRONIC HAZARDS: When heated to decomposition this compound emits toxic fumes of nitrogen oxides. (NTP, 1992)

### 4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Poisons A and B

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## SECTION 5: Fire-fighting measures

### 5.1 Suitable extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

### 5.2 Specific hazards arising from the chemical

Flash point data for this chemical are not available; however, it is probably combustible. (NTP, 1992)

### 5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

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## SECTION 6: Accidental release measures

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

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure

adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

## 6.2 Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

## 6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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# SECTION 7: Handling and storage

## 7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

## 7.2 Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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# SECTION 8: Exposure controls/personal protection

## 8.1 Control parameters

### Occupational Exposure limit values

Component	3-phenyl-L-alanine			
CAS No.	63-91-2			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m <sup>3</sup>	ppm	mg/m <sup>3</sup>
Latvia		5		
	Remarks			

### Biological limit values

no data available

## 8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

## 8.3 Individual protection measures, such as personal protective equipment (PPE)

### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Solid. Crystalline.
Colour	No data.
Odour	Slight
Melting point/freezing point	270 - 284 °C.
Boiling point or initial boiling point and boiling range	295 °C. Remarks: Sublimation.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	33°C(lit.)
Auto-ignition temperature	Remarks: The test item L-phenylalanine shows no self-heating up to the melting of the test item at a temperature of 165 °C. No self-ignition of the test item was observed.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	10 to 50 mg/mL at 77° F (NTP, 1992)
Partition coefficient n-octanol/water	log Pow = -1.52. Temperature: 20 °C.
Vapour pressure	0 mm Hg. Temperature: 25 °C.
Density and/or relative density	1.343 g/cm <sup>3</sup> . Temperature: 20 °C.; 1.343. Temperature: 20 °C.
Relative vapour density	no data available
Particle characteristics	no data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Water soluble. Aqueous solutions are weak acids.

### 10.2 Chemical stability

no data available

### 10.3 Possibility of hazardous reactions

L-PHENYLALANINE may be light sensitive. Acts as a weak acid in solution.

### 10.4 Conditions to avoid

no data available

### 10.5 Incompatible materials

no data available

### 10.6 Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /nitrogen oxides/.

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD50 - rat (female) -  $\geq 10\,000$  -  $\leq 16\,000$  mg/kg bw.

- Inhalation: no data available
- Dermal: no data available

#### **Skin corrosion/irritation**

no data available

#### **Serious eye damage/irritation**

no data available

#### **Respiratory or skin sensitization**

no data available

#### **Germ cell mutagenicity**

no data available

#### **Carcinogenicity**

no data available

#### **Reproductive toxicity**

no data available

#### **STOT-single exposure**

no data available

#### **STOT-repeated exposure**

no data available

#### **Aspiration hazard**

no data available

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

- Toxicity to fish: no data available
- Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - > 100 mg/L - 48 h.
- Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - > 100 mg/L - 72 h.
- Toxicity to microorganisms: no data available

### **12.2 Persistence and degradability**

AEROBIC: (DL)-Phenylalanine, present at 100 mg/L, exhibited 145 mg/L O<sub>2</sub> uptake over 3 hours using phenol-adapted soil compost or mud from a catalytic cracking plant waste lagoon in the Warburg test(1). Using a *Pseudomonas* sp., a proposed metabolic pathway for (L)-phenylalanine has been identified resulting in the formation of mandelic acid, benzylformic acid, benzaldehyde, benzoic acid, catechol, beta-ketoadipic acid, succinic acid, acetic acid, and formic acid(2).

### **12.3 Bioaccumulative potential**

An estimated BCF of 3 was calculated in fish for (L)-phenylalanine(SRC), using a log K<sub>ow</sub> of -1.38(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

### **12.4 Mobility in soil**

The K<sub>oc</sub> of (L)-phenylalanine is estimated as 54(SRC), using a log K<sub>ow</sub> of -1.38(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated K<sub>oc</sub> value suggests that (L)-phenylalanine is expected to have high mobility in soil. Amino acids are ionic over the entire pH range and tend to be cationic in acidic media, zwitterionic in neutral media, and anionic in basic media(4). The measured pK<sub>a1</sub> and pK<sub>a2</sub>

values for (L)-phenylalanine are 1.83 and 9.13, respectively(5), indicating that this compound will almost entirely exist in the ion form in the environment.

## 12.5 Other adverse effects

no data available

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## SECTION 13: Disposal considerations

### 13.1 Disposal methods

#### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

### 14.1 UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)      IMDG: Not dangerous goods. (For reference only, please check.)      IATA: Not dangerous goods. (For reference only, please check.)

### 14.2 UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)      IMDG: Not dangerous goods. (For reference only, please check.)      IATA: Not dangerous goods. (For reference only, please check.)

### 14.3 Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)      IMDG: Not dangerous goods. (For reference only, please check.)      IATA: Not dangerous goods. (For reference only, please check.)

### 14.4 Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)      IMDG: Not dangerous goods. (For reference only, please check.)      IATA: Not dangerous goods. (For reference only, please check.)

### 14.5 Environmental hazards

ADR/RID: No      IMDG: No      IATA: No

### 14.6 Special precautions for user

no data available

### 14.7 Transport in bulk according to IMO instruments

no data available

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## SECTION 15: Regulatory information

### 15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
3-phenyl-L-alanine	3-phenyl-L-alanine	63-91-2	200-568-1
European Inventory of Existing Commercial Chemical Substances			Listed.

(EINECS)	
EC Inventory	Listed.
United States Toxic Substances Control Act (TSCA) Inventory	Listed.
China Catalog of Hazardous chemicals 2015	Not Listed.
New Zealand Inventory of Chemicals (NZIoC)	Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Listed.
Vietnam National Chemical Inventory	Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)	Listed.
Korea Existing Chemicals List (KECL)	Listed.

## SECTION 16: Other information

### Information on revision

**Creation Date**                      July 15, 2019  
**Revision Date**                      July 15, 2019

### Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

### References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisys.com](mailto:sds@xixisys.com)**

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