

## SAFETY DATA SHEET

3,3-DIPHENYL-L-ALANINE

Page: 1

Compilation date: 17/11/2009

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Revision No: 1

### Section 1: Identification of the substance/mixture and of the company/undertaking

#### 1.1. Product identifier

**Product name:** 3,3-DIPHENYL-L-ALANINE

**CAS number:** 149597-92-2

**Product code:** OR14742

**Synonyms:** (2S)-2-AMINO-3,3-DIPHENYLPROPANOIC ACID

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

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

**Company name:** Apollo Scientific Ltd

Units 3 & 4

Parkway

Denton

Manchester

M34 3SG

UK

**Tel:** 0161 337 9971

**Fax:** 0161 336 6932

**Email:** david.tideswell@apolloscientific.co.uk

#### 1.4. Emergency telephone number

### Section 2: Hazards identification

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

**Classification under CLP:** Acute Tox. 2: H300

**Classification under CHIP:** T: R25

**Most important adverse effects:** Fatal if swallowed.

#### 2.2. Label elements

**Label elements:**

**Hazard statements:** H300: Fatal if swallowed.

**Signal words:** Danger

**Hazard pictograms:** GHS06: Skull and crossbones



**Precautionary statements:** P264: Wash thoroughly after handling.

# SAFETY DATA SHEET

3,3-DIPHENYL-L-ALANINE

Page: 2

P260: Do not breathe dust.

P280: Wear protective gloves/protective clothing/eye protection/face protection.

P309+311: IF exposed or if you feel unwell: Call a POISON CENTRE or doctor.

## 2.3. Other hazards

**PBT:** This product is not identified as a PBT/vPvB substance.

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 3,3-DIPHENYL-L-ALANINE

**CAS number:** 149597-92-2

## Section 4: First aid measures

### 4.1. Description of first aid measures

**Skin contact:** Remove all contaminated clothes and footwear immediately unless stuck to skin.

Drench the affected skin with running water for 10 minutes or longer if substance is still on skin. Transfer to hospital if there are burns or symptoms of poisoning.

**Eye contact:** Bathe the eye with running water for 15 minutes. Transfer to hospital for specialist examination.

**Ingestion:** Do not induce vomiting. If conscious, give half a litre of water to drink immediately. If unconscious and breathing is OK, place in the recovery position. Transfer to hospital as soon as possible.

**Inhalation:** Remove casualty from exposure ensuring one's own safety whilst doing so. Transfer to hospital as soon as possible.

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

**Skin contact:** There may be irritation and redness at the site of contact.

**Eye contact:** There may be pain and redness.

**Ingestion:** There may be soreness and redness of the mouth and throat. Severe poisoning can cause unconsciousness and severe and persistent nausea and vomiting. Severe poisoning can cause shock, unconsciousness and convulsions. Severe poisoning can cause vision to be blurred or blindness, severe headache and rapid gasping breathing.

**Inhalation:** There may be shortness of breath with a burning sensation in the throat. Absorption through the lungs can occur causing symptoms similar to those of ingestion. Nausea and stomach pain may occur.

**Delayed / immediate effects:** Immediate effects can be expected after short-term exposure.

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

**Immediate / special treatment:** Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.

[cont...]

# SAFETY DATA SHEET

3,3-DIPHENYL-L-ALANINE

Page: 3

## Section 5: Fire-fighting measures

### 5.1. Extinguishing media

**Extinguishing media:** Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the surrounding fire should be used. Use water spray to cool containers.

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

**Exposure hazards:** Toxic. In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NO<sub>x</sub>).

### 5.3. Advice for fire-fighters

**Advice for fire-fighters:** Wear self-contained breathing apparatus. Wear protective clothing to prevent contact with skin and eyes.

## Section 6: Accidental release measures

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

**Personal precautions:** Notify the police and fire brigade immediately. If outside keep bystanders upwind and away from danger point. Mark out the contaminated area with signs and prevent access to unauthorised personnel. Do not attempt to take action without suitable protective clothing - see section 8 of SDS. Do not create dust.

### 6.2. Environmental precautions

**Environmental precautions:** Do not discharge into drains or rivers.

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

**Clean-up procedures:** Clean-up should be dealt with only by qualified personnel familiar with the specific substance. Transfer to a closable, labelled salvage container for disposal by an appropriate method.

### 6.4. Reference to other sections

**Reference to other sections:** Refer to section 8 of SDS.

## Section 7: Handling and storage

### 7.1. Precautions for safe handling

**Handling requirements:** Avoid the formation or spread of dust in the air. Ensure there is sufficient ventilation of the area. Only use in fume hood.

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

**Storage conditions:** Store in a cool, well ventilated area. Keep container tightly closed.

**Suitable packaging:** Must only be kept in original packaging.

### 7.3. Specific end use(s)

**Specific end use(s):** No data available.

[cont...]

# SAFETY DATA SHEET

3,3-DIPHENYL-L-ALANINE

Page: 4

## Section 8: Exposure controls/personal protection

### 8.1. Control parameters

**Workplace exposure limits:** No data available.

### DNEL/PNEC Values

**DNEL / PNEC** No data available.

### 8.2. Exposure controls

**Engineering measures:** Ensure there is sufficient ventilation of the area.

**Respiratory protection:** Self-contained breathing apparatus must be available in case of emergency. Respiratory protective device with particle filter.

**Hand protection:** Protective gloves.

**Eye protection:** Safety glasses. Ensure eye bath is to hand.

**Skin protection:** Protective clothing.

## Section 9: Physical and chemical properties

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

**State:** Powder

**Colour:** Off-white

**Part.coeff. n-octanol/water:** logPow: 0.492

### 9.2. Other information

**Other information:** Decomposition Temperature: 240 °C

## Section 10: Stability and reactivity

### 10.1. Reactivity

**Reactivity:** Stable under recommended transport or storage conditions.

### 10.2. Chemical stability

**Chemical stability:** Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

**Hazardous reactions:** Hazardous reactions will not occur under normal transport or storage conditions.  
Decomposition may occur on exposure to conditions or materials listed below.

### 10.4. Conditions to avoid

**Conditions to avoid:** Heat.

### 10.5. Incompatible materials

**Materials to avoid:** Strong oxidising agents. Strong acids.

### 10.6. Hazardous decomposition products

**Haz. decomp. products:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NOx).

[cont...]

# SAFETY DATA SHEET

3,3-DIPHENYL-L-ALANINE

Page: 5

## Section 11: Toxicological information

### 11.1. Information on toxicological effects

#### Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 2)	ING	Based on test data

### Symptoms / routes of exposure

**Skin contact:** There may be irritation and redness at the site of contact.

**Eye contact:** There may be pain and redness.

**Ingestion:** There may be soreness and redness of the mouth and throat. Severe poisoning can cause unconsciousness and severe and persistent nausea and vomiting. Severe poisoning can cause shock, unconsciousness and convulsions. Severe poisoning can cause vision to be blurred or blindness, severe headache and rapid gasping breathing.

**Inhalation:** There may be shortness of breath with a burning sensation in the throat. Absorption through the lungs can occur causing symptoms similar to those of ingestion. Nausea and stomach pain may occur.

**Delayed / immediate effects:** Immediate effects can be expected after short-term exposure.

## Section 12: Ecological information

### 12.1. Toxicity

**Ecotoxicity values:** No data available.

### 12.2. Persistence and degradability

**Persistence and degradability:** No data available.

### 12.3. Bioaccumulative potential

**Bioaccumulative potential:** No data available.

### 12.4. Mobility in soil

**Mobility:** No data available.

### 12.5. Results of PBT and vPvB assessment

**PBT identification:** This product is not identified as a PBT/vPvB substance.

### 12.6. Other adverse effects

**Other adverse effects:** No data available.

## Section 13: Disposal considerations

### 13.1. Waste treatment methods

**Disposal operations:** MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL, STATE AND FEDERAL REGULATIONS

**Disposal of packaging:** Dispose of as special waste in compliance with local and national regulations Observe all federal, state and local environmental regulations.

[cont...]

# SAFETY DATA SHEET

3,3-DIPHENYL-L-ALANINE

Page: 6

**NB:** The user's attention is drawn to the possible existence of regional or national regulations regarding disposal.

## Section 14: Transport information

### 14.1. UN number

UN number: UN2811

### 14.2. UN proper shipping name

Shipping name: TOXIC SOLID, ORGANIC, N.O.S.

### 14.3. Transport hazard class(es)

Transport class: 6.1

### 14.4. Packing group

Packing group: III

### 14.5. Environmental hazards

Environmentally hazardous: No

Marine pollutant: No

### 14.6. Special precautions for user

Special precautions: No special precautions.

Tunnel code: E

Transport category: 2

## Section 15: Regulatory information

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

### 15.2. Chemical Safety Assessment

**Chemical safety assessment:** A chemical safety assessment has not been carried out for the substance or the mixture by the supplier.

## Section 16: Other information

### Other information

**Other information:** This safety data sheet is prepared in accordance with Commission Regulation (EU) No 453/2010.

\* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by decision tree approach. <http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?c=TOXTREE>

~ Data predicted using computational software ACD/ToxSuite v 2.95.1 Copyright 1994-2009 ACD/labs, Copyright 2001-2009 Pharma Algorithms, Inc, Advanced Chemistry Development, Inc (ACD/Labs). [http://www.acdlabs.com/products/pc\\_admet/tox/tox/](http://www.acdlabs.com/products/pc_admet/tox/tox/)

**Phrases used in s.2 and s.3:** H300: Fatal if swallowed.

R25: Toxic if swallowed.

[cont...]

## SAFETY DATA SHEET

3,3-DIPHENYL-L-ALANINE

Page: 7

**Legend to abbreviations:** PNEC = predicted no effect level  
DNEL = derived no effect level  
LD50 = median lethal dose  
LC50 = median lethal concentration  
EC50 = median effective concentration  
IC50 = median inhibitory concentration  
dw = dry weight  
bw = body weight  
cc = closed cup  
oc = open cup  
MUS = mouse  
GPG = guinea pig  
RBT = rabbit  
HAM = hamster  
HMN = human  
MAM = mammal  
PGN = pigeon  
IVN = intravenous  
SCU = subcutaneous  
SKN = skin  
DRM = dermal  
OCC = ocular/corneal  
PCP = physico-chemical properties

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