

A IN CENTRAL GLASS CO., LTE(5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-OXAZIN-2-ONE

Page: 1

Compilation date: 25/05/2016

Revision No: 1

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

#### 1.1. Product identifier

Product name: (5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-

OXAZIN-2-ONE

**CAS number:** 220077-24-7 **Product code:** OR304068

Synonyms: TERT-BUTYL (5S)-2-OXO-5-PHENYLMORPHOLINE-4-CARBOXYLATE

## 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: STOT SE 3: H335; Eye Irrit. 2: H319; Skin Irrit. 2: H315

Most important adverse effects: Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

## 2.2. Label elements

Label elements:

Hazard statements: H315: Causes skin irritation.

H319: Causes serious eye irritation.H335: May cause respiratory irritation.

Signal words: Warning

Hazard pictograms: GHS07: Exclamation mark



(5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-OXAZIN-2-ONE

Page: 2

**Precautionary statements:** P271: Use only outdoors or in a well-ventilated area.

P261: Avoid breathing dust.

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

#### 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: (5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-

**OXAZIN-2-ONE** 

CAS number: 220077-24-7

#### 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. Wash

immediately with plenty of soap and water.

**Eye contact:** Bathe the eye with running water for 15 minutes. Consult a doctor.

Ingestion: Wash out mouth with water. Consult a doctor.

Inhalation: Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a

doctor.

### 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 irritation and redness. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest. Exposure may

cause coughing or wheezing.

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

# 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.

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

**Exposure hazards:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides

(NOx).

## 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.

(5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-OXAZIN-2-ONE

Page: 3

#### Section 6: Accidental release measures

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

Personal precautions: Refer to section 8 of SDS for personal protection details. If outside do not approach from

downwind. 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

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: Transfer to a closable, labelled salvage container for disposal by an appropriate

method.

#### 6.4. Reference to other sections

## Section 7: Handling and storage

#### 7.1. Precautions for safe handling

Handling requirements: Avoid direct contact with the substance. Ensure there is sufficient ventilation of the area.

Do not handle in a confined space. Avoid the formation or spread of dust in the air. 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. Recommended

storage temp 2-8 ℃.

Suitable packaging: Must only be kept in original packaging.

#### 7.3. Specific end use(s)

Specific end use(s): No data available.

## 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.

(5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-OXAZIN-2-ONE

Page: 4

Skin protection: Protective clothing.

### Section 9: Physical and chemical properties

## 9.1. Information on basic physical and chemical properties

State: Solid

Colour: Off-white

Also soluble in: Most organic solvents.

Melting point/range ℃: 86-88

#### 9.2. Other information

Other information: No data available.

## 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.

## 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).

## **Section 11: Toxicological information**

# 11.1. Information on toxicological effects

#### Relevant hazards for substance:

| Hazard                        | Route | Basis                 |
|-------------------------------|-------|-----------------------|
| Skin corrosion/irritation     | DRM   | Hazardous: calculated |
| Serious eye damage/irritation | OPT   | Hazardous: calculated |
| STOT-single exposure          | INH   | Hazardous: calculated |

#### Symptoms / routes of exposure

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

**Eye contact:** There may be irritation and redness. The eyes may water profusely.

(5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-OXAZIN-2-ONE

Page: 5

**Ingestion:** There may be soreness and redness of the mouth and throat.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest. Exposure may

cause coughing or wheezing.

### 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: Transfer to a suitable container and arrange for collection by specialised disposal

company. 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.

NB: The user's attention is drawn to the possible existence of regional or national

regulations regarding disposal.

#### **Section 14: Transport information**

**Transport class:** This product does not require a classification for transport.

## **Section 15: Regulatory information**

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

Specific regulations: Not applicable.

### 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.

(5S)-N-TERT-BUTYLOXYCARBONYL-3,4,5,6-TETRAHYDRO-5-PHENYL-4(H)-1,4-OXAZIN-2-ONE

Page: 6

#### 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. The OECD QSAR-Toolbox for grouping chemicals into categories. Developed by LMC bulgaria.

http://echa.europa.eu/support/oecd-qsar-toolbox

~ 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/

Phrases used in s.2 and s.3: H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

Legal disclaimer: The material is intended for research purposes only and should be handled exclusively by those who have been fully trained in safety, laboratory and chemical handling procedures. The above information is believed to be correct to the best of our knowledge. The above information is believed to be correct to the best of our knowledge at the date of its publication, but should not be considered to be all inclusive. It should be used only as a guide for safe handling, storage, transportation and disposal. We cannot guarantee that the hazards detailed in this document are the only hazards that exist for this product. This is not a warranty and Apollo Scientific Ltd shall not be held liable for any damage resulting from handling or from contact with the above product.