

**SAFETY DATA SHEET**

3,4-DIHYDRO-2H-1,5-BENZODIOXEPINE-7-CARBONYL CHLORIDE

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Compilation date: 10/2/2004

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Revision No: 2

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

**1.1. Product identifier**

**Product name:** 3,4-DIHYDRO-2H-1,5-BENZODIOXEPINE-7-CARBONYL CHLORIDE

**CAS number:** 306934-86-1

**Product code:** OR23205

**Synonyms:** 7-(CHLOROCARBONYL)-3,4-DIHYDRO-2H-1,5-BENZODIOXEPINE  
7-(CHLOROFORMYL)-3,4-DIHYDRO-2H-1,5-BENZODIOXEPINE

**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 CHIP:** C: R34; Xi: R41

**Classification under CLP:** Skin Corr. 1B: H314; Eye Dam. 1: H318

**Most important adverse effects:** Causes burns. Risk of serious damage to eyes.

**2.2. Label elements**

**Label elements under CLP:**

**Hazard statements:** H314: Causes severe skin burns and eye damage.

H318: Causes serious eye damage.

**Signal words:** Danger

**Hazard pictograms:** GHS05: Corrosion



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**Precautionary statements:** P280: Wear protective gloves/protective clothing/eye protection/face protection.  
P309+311: IF exposed or if you feel unwell: Call a POISON CENTER or doctor.

### Label elements under CHIP:

**Hazard symbols:** Corrosive.



**Risk phrases:** R34: Causes burns.

R41: Risk of serious damage to eyes.

**Safety phrases:** S24/25: Avoid contact with skin and eyes.

S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S28: After contact with skin, wash immediately with plenty of.

S36/37/39: Wear suitable protective clothing, gloves and eye / face protection.

S45: In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

### 2.3. Other hazards

**PBT:** This substance is not identified as a PBT substance.

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 3,4-DIHYDRO-2H-1,5-BENZODIOXEPINE-7-CARBONYL CHLORIDE

## 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:** Wash out mouth with water. Do not induce vomiting. Give 1 cup of water to drink every 10 minutes. If unconscious, check for breathing and apply artificial respiration if necessary. 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. If unconscious and breathing is OK, place in the recovery position. If conscious, ensure the casualty sits or lies down. If breathing becomes bubbly, have the casualty sit and provide oxygen if available. Transfer to hospital as soon as possible.

[cont...]

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

**Skin contact:** Blistering may occur. Progressive ulceration will occur if treatment is not immediate.

**Eye contact:** Corneal burns may occur. May cause permanent damage.

**Ingestion:** Corrosive burns may appear around the lips. Blood may be vomited. There may be bleeding from the mouth or nose.

**Inhalation:** There may be shortness of breath with a burning sensation in the throat. 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. Use water spray to cool containers.

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

**Exposure hazards:** Corrosive. In combustion emits toxic fumes. Carbon oxides. Hydrogen chloride (HCl).

### 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

## 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.

[cont...]

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

**Storage conditions:** Store in cool, well ventilated area. Keep container tightly closed. Air sensitive. Moisture sensitive. Store under Argon.

**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:** Not applicable.

### 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:** Tightly fitting safety goggles. 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:** Solid

**Oxidising:** Non-oxidising (by EC criteria)

**Melting point/range °C:** 29-33

### 9.2. Other information

**Other information:** Not applicable.

## 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. Air. Moist air.

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## 10.5. Incompatible materials

**Materials to avoid:** Bases. Strong oxidising agents. Alcohols. Amines. Water.

## 10.6. Hazardous decomposition products

**Haz. decomp. products:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Hydrogen chloride (HCl).

## Section 11: Toxicological information

### 11.1. Information on toxicological effects

#### Relevant hazards for substance:

Hazard	Route	Basis
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data

### Symptoms / routes of exposure

**Skin contact:** Blistering may occur. Progressive ulceration will occur if treatment is not immediate.

**Eye contact:** Corneal burns may occur. May cause permanent damage.

**Ingestion:** Corrosive burns may appear around the lips. Blood may be vomited. There may be bleeding from the mouth or nose.

**Inhalation:** There may be shortness of breath with a burning sensation in the throat. Exposure may cause coughing or wheezing.

## Section 12: Ecological information

### 12.1. Toxicity

**Ecotoxicity values:** Not applicable.

### 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 substance is not identified as a PBT substance.

### 12.6. Other adverse effects

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

## Section 13: Disposal considerations

[cont...]

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### 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.

**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:** UN3261

### 14.2. UN proper shipping name

**Shipping name:** CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.

### 14.3. Transport hazard class(es)

**Transport class:** 8

### 14.4. Packing group

**Packing group:** III

### 14.5. Environmental hazards

**Environmentally hazardous:** No

**Marine pollutant:** No

### 14.6. Special precautions for user

**Tunnel code:** E

**Transport category:** 3

## 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-

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**Phrases used in s.2 and 3:** H314: Causes severe skin burns and eye damage.

H318: Causes serious eye damage.

R34: Causes burns.

R41: Risk of serious damage to eyes.

**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.