1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product identifiers

Product Name: ODQ
Catalog Number: 0880
CAS Number: 41443-28-1
IUPAC Name: 1H-[1,2,4]Oxadiazolo[4,3-a]quinoxalin-1-one

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

Identified Uses: Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company: Tocris Bioscience
The Watkins Building,
Atlantic Road,
Bristol, BS11 9QD, UK

Telephone: + 44 (0)117 916-3333
Fax: + 44 (0)117 916-3344
Internet: www.tocris.com
E-mail address: customerservice@tocris.co.uk

1.4 Emergency Telephone number

Emergency Tel: + 44 (0)117 916-3333 (09.00 - 17.00 GMT)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 [GHS/CLP]
Skin Corrosion/Irritation - Category 2
Serious eye damage/eye irritation - Category 2
Specific Target Organ Toxicity, SE, respiratory tract irritation - Category 3

Classification according to EU Directives DSD 67/548/EEC or DPD 1999/45/EC
Irritating to eyes.
Irritating to respiratory system.
Irritating to skin

2.2 Label elements

Labeling according to Regulation (EC) No 1272/2008 [CLP]

Pictogram(s):

Signal word: Warning

Hazard statement(s):
H315 Causes skin irritation
H319 Causes serious eye irritation
H335 May cause respiratory irritation

Precautionary statement(s):
P260 Do not breathe dust/fume/gas/mist/vapours/spray
P264 Wash hands thoroughly after handling
P280 Wear protective gloves/protective clothing/eye protection/face protection
P302+352 IF ON SKIN: Wash with soap and water
P304+340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
P305+351+338 IF IN EYES: Rinse continuously with water for several minutes. Remove contact lenses if present and easy to do so - continue rinsing
P333+313 If skin irritation or a rash occurs: Get medical advice/attention

According to European Directive 67/548/EEC as amended

Hazard symbol(s):

R-phrase(s):
R36 Irritating to eyes
R37 Irritating to respiratory system
R38 Irritating to skin

S-phrase(s):
S22 Do not breathe dust
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 water
S36/37/39 Wear suitable protective clothing, gloves and eye/face protection
S63 In case of accident by inhalation: remove casualty to fresh air and keep at rest

2.3 Other hazards - none
3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
Product Name: ODQ
Formula: C₉H₅N₃O₂ Molecular Weight: 187.16
CAS Number: 41443-28-1

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a doctor and show this safety data sheet.

If inhaled
Remove to fresh air and monitor breathing. If breathing becomes difficult, give oxygen. If breathing stops, give artificial respiration. Consult a doctor.

In case of skin contact
Immediately wash skin with copious amounts of soap and water for at least 15 minutes. Remove contaminated clothing and shoes and wash before reuse. Consult a doctor.

In case of eye contact
Flush with copious amounts of water for at least 15 minutes. Consult a doctor.

If swallowed
Rinse mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Consult a doctor.

4.2 Most important symptoms and effects, both acute and delayed
To the best of our knowledge, the chemical, physical and toxicological properties have not been thoroughly investigated.

4.3 Indication of immediate medical attention and special treatment needed
Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
In combustion, may emit toxic fumes.

5.3 Precautions for fire-fighters
Wear suitable protective clothing to prevent contact with skin and eyes and self-contained breathing apparatus.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Do not take action without suitable protective clothing - see section 8 of SDS. Evacuate personnel to safe areas. Ensure adequate ventilation. Avoid breathing vapors, mist, dust or gas.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Cover spillage with suitable absorbent material. Using non-spark tools, sweep up material and place in an appropriate container. Decontaminate spill site with 10% caustic solution and ventilate area until after disposal is complete. Hold all material for appropriate disposal as described under section 13 of SDS.

6.4 Reference to other sections
For required PPE see section 8. For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Use in a chemical fume hood, with air supplied by an independent system. Avoid inhalation, contact with eyes, skin and clothing. Avoid the formation of dust and aerosols. Use in a well-ventilated area. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

7.2 Conditions for safe storage, including any incompatibilities.
Store in cool, well-ventilated area. Keep away from direct sunlight. Keep container tightly sealed until ready for use. Recommended storage temperature: Desiccate at +4°C

7.3 Specific end uses
Use in a laboratory fume hood where possible. Refer to employer's COSHH risk assessment.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters
Components with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

**Appropriate engineering controls**
Use in a fume hood where applicable. Ensure all engineering measures described under section 7 of SDS are in place. Ensure laboratory is equipped with a safety shower and eye wash station.

**Personal protective equipment**

**Eye/face protection**
Use appropriate safety glasses.

**Skin protection**
Use appropriate chemical resistant gloves (minimum requirement use standard BS EN 374:2003). Gloves should be inspected before use. Wash and dry hands thoroughly after handling.

**Body protection**
Wear appropriate protective clothing.

**Respiratory protection**
If risk assessment indicates necessary, use a suitable respirator.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Yellow solid</td>
</tr>
<tr>
<td>Odor</td>
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</tr>
<tr>
<td>Odor threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>No data available</td>
</tr>
<tr>
<td>Boiling point/ range</td>
<td>No data available</td>
</tr>
<tr>
<td>Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
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</tr>
<tr>
<td>Upper / lower flammability or</td>
<td>No data available</td>
</tr>
<tr>
<td>explosive limits</td>
<td></td>
</tr>
<tr>
<td>Vapor pressure</td>
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</tr>
<tr>
<td>Vapor density</td>
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</tr>
<tr>
<td>Relative density</td>
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</tr>
<tr>
<td>Solubility(ies)</td>
<td>Soluble to 20 mM in ethanol and to 100 mM in DMSO</td>
</tr>
<tr>
<td>Partition coefficient</td>
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</tr>
<tr>
<td>Auto-ignition temperature</td>
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</tr>
<tr>
<td>Decomposition temperature</td>
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<tr>
<td>Viscosity</td>
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<tr>
<td>Explosive properties</td>
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</tr>
<tr>
<td>Oxidising properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
Stable under recommended transport or storage conditions.

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of 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
Heat, moisture.

10.5 Incompatible materials
Strong acids/alkalis, strong oxidising/reducing agents.

10.6 Hazardous decomposition products
In combustion may emit toxic fumes. No known decomposition information.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

**Acute Toxicity**
No data available

**Skin corrosion/irritation**
Classified based on available data

**Serious eye damage/irritation**
Classified based on available data

**Respiratory or skin sensitization**
Classified based on available data

**Germ cell mutagenicity**
Classified based on available data

**Carcinogenicity**
Classified based on available data
Reproductive toxicity
Classified based on available data

Specific target organ toxicity - single exposure
Classified based on available data

Specific target organ toxicity - repeated exposure
Classified based on available data

Aspiration hazard
Classified based on available data

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

Ingestion: There may be soreness and redness of the mouth and throat. There may be difficulty swallowing. Nausea and stomach pain may occur. There may be irritation of the throat.

Skin: There may be mild irritation at the site of contact. The skin will become dry and flaky. An itchy rash may occur at the site of contact. Irritation or pain may occur at the site of contact.

Eyes: There may be pain and redness. There may be severe pain. The eyes may water profusely. The vision may become blurred. May cause permanent damage.

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

Additional Information
RTECS No: RO0913150
Exposure may cause irritation of eyes, mucous membranes, upper respiratory tract and skin.
To the best of our knowledge, the chemical, physical and toxicological properties have not been fully investigated

12. ECOLOGICAL INFORMATION

12.1 Toxicity
No data available

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
No data available

12.6 Other adverse effects
May be harmful to the aquatic environment.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Transfer to a suitable container and arrange for collection by specialized disposal company in accordance with National legislation.

Contaminated packaging
Dispose of in a regulated landfill site or other method for hazardous or toxic wastes in accordance with National legislation.

14. TRANSPORT INFORMATION

Classified according to the criteria of the UN Model Regulations as reflected in the IMDG Code, ADR, RID and IATA.

14.1 UN-Number
Does not meet the criteria for classification as hazardous for transport.

14.2 UN proper shipping name
Does not meet the criteria for classification as hazardous for transport.

14.3 Transport hazard class(es)
Does not meet the criteria for classification as hazardous for transport.

14.4 Packaging group
Does not meet the criteria for classification as hazardous for transport.

14.5 Environmental hazards
This product is not classified as environmentally hazardous according to the UN Model Regulations, nor a marine pollutant according to the IMDG Code.

14.6 Special precautions for users
No data available

15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulation (EC) No. 453/2010.
15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture
No data available

15.2 Chemical safety assessment
A Chemical Safety Assessment has not been made for this product.

16. OTHER INFORMATION

Further Information
Copyright © 2016 Tocris Bioscience. This company shall not be held liable for any damage resulting from handling or from contact with the above product. This material must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The above information is believed to be correct but does not purport to be all inclusive and should be used as a guide only for experienced personnel. Always consult your safety advisor and follow appropriate local and national safety legislature. The absence of warning must not, under any circumstance, be taken to mean that no hazard exists.

End of safety data sheet