

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

**1.1 Product identifiers**

Product Name: Ketoconazole  
 Catalog Number: 1103  
 CAS Number: 65277-42-1 EC Number: 265-667-4  
 Index Number: 613-283-00-6  
 IUPAC Name: *cis*-1-Acetyl-4-[4-[[2-(2,4-dichlorophenyl)-2-(1*H*-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl] methoxy] phenyl]piperazine

**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 Telephone: + 44 (0)117 916-3333  
 The Watkins Building, Fax: + 44 (0)117 916-3344  
 Atlantic Road, Internet: [www.tocris.com](http://www.tocris.com)  
 Bristol, BS11 9QD, UK E-mail address: [info@bio-techne.com](mailto:info@bio-techne.com)

**1.4 Emergency Telephone number**

For chemical emergency spill, leak, fire, exposure, or accident call CHEMTREC day or night:  
 Within USA and Canada: 1-800-424-9300. Outside USA and Canada: +1 703-527-3887 (collect calls accepted).

**2. HAZARDS IDENTIFICATION**

**2.1 Classification of the substance or mixture**

**Classification according to Regulation (EC) No 1272/2008 [GHS/CLP]**

Acute Toxicity, oral - Category 3  
 Specific Target Organ Toxicity, repeated exposure - Category 2  
 Acute, Aquatic Toxicity - Category 1  
 Chronic, Aquatic Toxicity - Category 1

**2.2 Label elements**

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

Pictogram(s):



Signal word: Danger

Hazard statement(s):

H301 Toxic if swallowed  
 H373 May cause damage to organs through prolonged or repeated exposure  
 H400 Very toxic to aquatic life  
 H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s):

P260 Do not breathe dust/fume/gas/mist/vapours/spray  
 P264 Wash hands thoroughly after handling  
 P273 Avoid release to the environment  
 P301+310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
 P314 Get medical advice/attention if you feel unwell

**2.3 Other hazards - none**

**3. COMPOSITION/INFORMATION ON INGREDIENTS**

**3.1 Substances**

Product Name: Ketoconazole  
 Formula: C<sub>26</sub>H<sub>28</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>4</sub> Molecular Weight: 531.44  
 CAS Number: 65277-42-1 EC Number: 265-667-4  
 Index Number: 613-283-00-6

**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.

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**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.

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**6. ACCIDENTIAL 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. Sweep up material and place in an appropriate container. 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.

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**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.

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**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.

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## **9. PHYSICAL AND CHEMICAL PROPERTIES**

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

Appearance	White solid	Vapor pressure	No data available
Odor	No data available	Vapor density	No data available
Odor threshold	No data available	Relative density	No data available
pH	No data available	Solubility(ies)	Soluble to 50 mM in ethanol and to 75 mM in DMSO
Melting / freezing point	No data available	Partition coefficient	No data available
Boiling point / range	No data available	Auto-ignition temperature	No data available
Flash point	No data available	Decomposition temperature	No data available
Evaporation rate	No data available	Viscosity	No data available
Flammability (solid, gas)	No data available	Explosive properties	No data available
Upper / lower flammability or explosive limits	No data available	Oxidising properties	No data available

### **9.2 Other safety information**

No data available

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## **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.

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## **11. TOXICOLOGICAL INFORMATION**

### **11.1 Information on toxicological effects**

#### **Acute Toxicity**

ORL-RAT LD50: 166mg/kg; ORL-MAN LDLo: 45mg/kg; ORL-WMN LDLo: 412mg/kg; ORL-WMN LDLo: 264mg/kg; ORL-CHD TDLo: 450mg/kg; ORL-MAN TDLo: 49mg/kg; ORL-WMN TDLo: 60mg/kg; IPR-RAT LD50: 1474mg/kg; SCU-RAT LD50: >2400mg/kg; IVN-RAT LD50: 86mg/kg

#### **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. Absorption through the lungs can occur causing symptoms similar to those of ingestion. Severe poisoning causes severe shortness of breath and shock, with blueness of the lips, tongue, ears, face, hands and feet.

**Ingestion:** There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. Blood may be vomited. There may be vomiting and diarrhea. There may be loss of consciousness. Severe poisoning can cause unconsciousness and severe and persistent nausea and vomiting. Severe poisoning can cause shock, unconsciousness and convulsions.

**Skin:** Irritation or pain may occur at the site of contact. There may be redness or whiteness of the skin in the area of exposure. Absorption through the skin may be fatal.

**Eyes:** There may be pain and redness. The vision may become blurred. The eyes may water profusely. Absorption through the eye may cause effects similar to skin and/or ingestion.

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

**Additional Information**

RTECS No: TK79123000

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

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**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**

Very toxic to aquatic life. Very toxic to aquatic life with long lasting effects.

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**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.

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**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**

UN2811

**14.2 UN proper shipping name**

Toxic solid, organic, n.o.s. (Ketoconazole)

**14.3 Transport hazard class(es)**

6.1

**14.4 Packaging group**

III

**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

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## 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

#### California Proposition 65

Not applicable

### 15.2 Chemical safety assessment

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

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## 16. OTHER INFORMATION

### Further Information

Copyright © 2020 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