

# Ketoconazole SDS/MSDS (Safety Data Sheet)

## 1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

\* Product Name: Ketoconazole

\* Catalog Number: S1353

\* CAS Number: 65277-42-1

\* IUPAC Name: 1-(4-(4-(((2R,4S)-2-((1H-imidazol-1-yl)methyl)-2-(2,4-dichlorophenyl)-1,3-dioxolan-4-yl)methoxy)phenyl)piperazin-1-yl)ethanone

Relevant identified uses and uses advised against

\* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

\* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

\* Company: Selleck Chemicals

\* TollFree: +1 877 796-6397

\* Tel: +1 832 582-8158

\* Fax: +1 832 582-8590

Emergency telephone number

\* Emergency phone #: +1 832 582-8158

## 2. HAZARDS IDENTIFICATION

### 2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Acute toxicity (oral): Category 3. H301

Reproductive toxicity: Category 1. H360

Not classified. H360F

Specific target organ toxicity (repeated exposure): Category 2. H373

Acute aquatic toxicity: Category 1. H400

Chronic aquatic toxicity: Category 1. H410

### 2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

H301: Toxic if swallowed

H360: May damage fertility or the unborn child

H360F: May damage fertility

H373: May causes damage to organs through prolonged or repeated exposure

H400: Very toxic to aquatic life

H410: Very toxic to aquatic life with long lasting effects

|                                   |                                                                                                                                                                                                                                                                                                                                                                                                                     |
|-----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Precautionary statement(s)</b> | None.                                                                                                                                                                                                                                                                                                                                                                                                               |
| <b>Prevention</b>                 | <p>P203: Obtain, read and follow all safety instructions before use.</p> <p>P260: Do not breathe dust/fume/gas/mist/vapors/spray.</p> <p>P264: Wash hands thoroughly after handling.</p> <p>P270: Do not eat, drink or smoke when using this product.</p> <p>P273: Avoid release to the environment.</p> <p>P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.</p> |
| <b>Response</b>                   | <p>P301+P316: IF SWALLOWED: Get emergency medical help immediately.</p> <p>P318: if exposed or concerned, get medical advice.</p> <p>P319: Get medical help if you feel unwell.</p> <p>P321: Specific treatment (see information on this label and safety datasheet)).</p> <p>P330: Rinse mouth.</p> <p>P391: Collect spillage.</p>                                                                                 |
| <b>Storage</b>                    | P405: Store locked up.                                                                                                                                                                                                                                                                                                                                                                                              |
| <b>Disposal</b>                   | P501: P501 Dispose of contents/ container to an approved waste disposal plant.                                                                                                                                                                                                                                                                                                                                      |

### 2.3 Other hazards

None.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Product name: Ketoconazole

CAS Number: 65277-42-1

PubChem CID: 47576

Molecular formula: C<sub>26</sub>H<sub>28</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>4</sub>

Molecular weight: 531.4 g/mol

IUPAC name: 1-[4-[4-[(2S,4R)-2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazin-1-yl]ethanone

### 3.2 Mixtures

Not applicable (pure substance).

## 4. FIRST-AID MEASURES

### 4.1 Description of first aid measures

Inhalation: Fresh air, rest.

Skin contact: Rinse and then wash skin with water and soap.

Eye contact: Rinse with plenty of water (remove contact lenses if easily possible).

Ingestion: Rinse mouth. Give a slurry of activated charcoal in water to drink. Refer immediately for medical attention.

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

See Section 11 (Toxicological Information).

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

Treat symptomatically. Contact a poison control center or physician for severe exposure.

### **5. FIRE-FIGHTING MEASURES**

#### **5.1 Extinguishing media**

Suitable: Water spray, dry chemical, carbon dioxide (CO<sub>2</sub>), alcohol-resistant foam.

Unsuitable: None known.

#### **5.2 Specific hazards arising from the substance or mixture**

In case of fire in the surroundings, use appropriate extinguishing media.

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

Advice for firefighters: Wear self contained breathing apparatus for fire fighting if necessary.

#### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

### **6. ACCIDENTAL RELEASE MEASURES**

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

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

WARNING: Highly toxic — only trained personnel should handle spills.

#### **6.2 Environmental precautions**

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

#### **6.3 Methods and materials for containment and cleaning up**

Personal protection: filter respirator for organic gases and particulates adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Accidental Release Measures. Personal precautions, protective equipment and emergency procedures: Wear respiratory protection. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

SRP: Expired or waste pharmaceuticals shall carefully take into consideration applicable DEA, EPA, and FDA regulations. It is not appropriate to dispose by flushing the pharmaceutical down the toilet or discarding to trash. If possible return the pharmaceutical to the manufacturer for proper disposal being careful to properly label and securely package the material. Alternatively, the waste pharmaceutical shall be labeled, securely packaged and transported by a state licensed medical waste contractor to dispose by burial in a licensed hazardous or toxic waste landfill or incinerator.

SRP: At the time of review, regulatory criteria for small quantity disposal are subject to significant revision, however, household quantities of waste pharmaceuticals may be managed as follows: Mix with wet cat litter or coffee grounds, double bag in plastic, discard in trash.

Waste treatment methods. Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Contaminated packaging: Dispose of as unused product.

Appropriate engineering controls: Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Precautions for safe handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed.

Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

## **7. HANDLING AND STORAGE**

### **7.1 Precautions for safe handling**

Provision to contain effluent from fire extinguishing. Well closed. Separated from food and feedstuffs. Store in an area without drain or sewer access.

Store at controlled room temperature 15 deg - 25 °C (59 deg - 77 °F). Protect from moisture.

Ketoconazole topical cream should be stored at a temperature less than 25 °C and should not be frozen. The cream should not be stored at high temperatures (eg, warmer than 37 °C), since creams generally separate at these temperatures. Ketoconazole 2% shampoo should be stored at temperatures not exceeding 25 °C and should be protected from light; the 1% shampoo should be stored between 2-30 °C and should be protected from light and freezing.

Conditions for safe storage, including any incompatibilities: Keep container tightly closed in a dry and well-ventilated place. Recommended storage temperature: 2 - 8 °C.

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

Provision to contain effluent from fire extinguishing. Well closed. Separated from food and feedstuffs. Store in an area without drain or sewer access.

Store at controlled room temperature 15 deg - 25 °C (59 deg - 77 °F). Protect from moisture.

Ketoconazole topical cream should be stored at a temperature less than 25 °C and should not be frozen. The cream should not be stored at high temperatures (eg, warmer than 37 °C), since creams generally separate at these temperatures. Ketoconazole 2% shampoo should be stored at temperatures not exceeding 25 °C and should be protected from light; the 1% shampoo should be stored between 2-30 °C and should be protected from light and freezing.

Conditions for safe storage, including any incompatibilities: Keep container tightly closed in a dry and well-ventilated place. Recommended storage temperature: 2 - 8 °C.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

## **8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1 Exposure controls**

#### 8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

#### 8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

### **8.2 Individual protection measures**

#### 8.2.1 Eye/face protection

Wear safety glasses with side shields.

#### 8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

#### 8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

#### 8.2.4 Thermal hazards

Not applicable.

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

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

a) Appearance: Solid

b) Odor: No data available

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 146 °C

f) Initial boiling point and boiling range: No data available

g) Flash point: No data available

h) Evaporation rate: No data available

i) Flammability (solid, gas): No data available

j) Upper/lower flammability or explosive limits: No data available

k) Vapor pressure: Vapor pressure, Pa at 25 °C: (negligible)

l) Vapor density: No data available

m) Relative density: No data available

n) Water solubility: 0.0866 mg/L

o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 4.3

p) Auto-ignition temperature: No data available

q) Decomposition temperature: No data available

- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

## 9.2 Other information

Topological Polar Surface Area (TPSA): 69.1 Å<sup>2</sup>  
Complexity: 735

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

### 10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.  
Avoid strong oxidizing agents, strong acids, and strong bases.

### 10.5 Incompatible materials

Incompatible materials: Strong oxidizing agents.

### 10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), Hydrogen chloride (HCl).  
See also Section 5 (Fire-fighting measures) for combustion products.

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity:

No acute toxicity data available.

#### Skin corrosion/irritation:

No data available.

#### Serious eye damage/eye irritation:

No data available.

#### Respiratory or skin sensitization:

No data available.

#### Germ cell mutagenicity:

No data available.

#### Carcinogenicity:

No data available.

**Reproductive toxicity:**

May damage fertility or the unborn child (H360).

**Specific target organ toxicity (single exposure):**

H373

**Specific target organ toxicity (repeated exposure):**

No data available.

**Aspiration hazard:**

No data available.

## 11.2 Additional information

**Carcinogen classification:**

No indication of carcinogenicity to humans (not listed by IARC).

**Exposure routes:**

The substance can be absorbed into the body by ingestion.

Oral (L1908) ; topical (L1908)

**Signs and symptoms of exposure:**

Cough.

Redness.

Nausea. Headache. Dizziness. Vomiting. Diarrhoea.

Side effects of the potential hepatotoxicity of Ketoconazole include abdominal pain or tenderness, clay-colored stools, dark urine, decreased appetite, fever, headache, itching, loss of appetite, nausea and vomiting, skin rash, swelling of the feet or lower legs, unusual tiredness or weakness, and yellow eyes or skin. (L1536)

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

EC50; Species: Daphnia magna (Water Flea) age <24 hr neonate; Conditions: freshwater, static, 20 °C; Concentration: 8100 ug/L for 24 hr (95% confidence interval: 4600-10800 ug/L); Effect: intoxication, immobilization /100% purity/

EC50; Species: Daphnia magna (Water Flea) age <24 hr neonate; Conditions: freshwater, static, 20 °C; Concentration: 1510 ug/L for 48 hr (95% confidence interval: 1160-1910 ug/L); Effect: intoxication, immobilization /100% purity/

/AQUATIC SPECIES/ The use of N-substituted imidazoles is widespread, and imidazole and triazole fungicides have been detected in the aquatic environment and shown to bioaccumulate in fish. ...The effects of the model imidazole, ketoconazole, on drug-metabolizing cytochrome P450 (CYP) forms /were investigated;/ ... focused on cytochrome P4501A (CYP1A) and cytochrome P4503A (CYP3A) expression and activities in juvenile rainbow trout and in adult killifish. The CYP1A expression (mRNA, protein) and activity was induced in rainbow trout, whereas in killifish no effect of ketoconazole on CYP1A protein expression was observed. A biphasic dose-response relationship was observed between ketoconazole exposure and hepatic CYP1A-mediated ethoxyresorufin O-deethylase (EROD) activity in rainbow trout in vitro and in vivo, implying that higher doses of ketoconazole inhibit CYP1A activities. Slight induction of CYP3A protein levels was observed in rainbow trout exposed in vivo to ketoconazole. However, the CYP3A-mediated benzyloxy-4-[trifl

### 12.2 Persistence and degradability

No data available.

**12.3 Bioaccumulative potential**

Log P (n-octanol/water): 4.3

Potential for bioaccumulation exists (Log P > 3).

**12.4 Mobility in soil**

No data available.

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available.

**12.6 Other adverse effects**

This substance is classified as hazardous to the aquatic environment.

**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

**14. TRANSPORT INFORMATION****14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

**14.2 UN proper shipping name**

Not subject to transport regulations (small quantities for research use).

**14.3 Transport hazard class(es)**

Class 6.1

**14.4 Packing group**

Packing group III

**14.5 Environmental hazards**

Marine pollutant: Yes (classified as environmentally hazardous per GHS).

**14.6 Special precautions for user**

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

**14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code**

Not applicable.

**15. REGULATORY INFORMATION****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Not available in public databases.

**SARA 302 Components:**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components:**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards:**

Acute (short-term) health hazard

Chronic (long-term) health hazard

Environmental hazard

**Massachusetts Right To Know Components:**

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

**Pennsylvania Right To Know Components:**

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

**New Jersey Right To Know Components:**

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

**California Prop. 65 Components:**

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

**Other regulatory listings:**

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Reproductive Toxicity Authoritative List - EC Annex VI CMRs - Cat. 1B Report - if used as a fragrance or flavor ingredient
  - FDA Requirements: The Approved Drug Products with Therapeutic Equivalence Evaluations identifies currently marketed prescription drug products, including ketoconazole, approved on the basis of safety and effectiveness by FDA under sections 505 of the Federal Food, Drug, and Cosmetic Act.
- The Approved Drug Products wi

**15.2 Chemical safety assessment**

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

**16. OTHER INFORMATION**

Revision Date: 2026/09/08

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product. Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.