

## (±)-Ketoconazole-d<sub>4</sub> (piperazine-3,3,5,5-d<sub>4</sub>) (*cis*-isomers)

### Section 1. Chemical product and company identifications

**Product code:** D-7488

**Chemical formula:** C<sub>26</sub>H<sub>24</sub>D<sub>4</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>4</sub>

**CAS:** 1398065-75-2

**CAS (unlabelled):** 65277-42-1

**Synonyms:** (±)-*cis*-1-Acetyl-4-[[[2-(2,4-dichlorophenyl)-2-(1*H*-imidazol-1-ylmethyl)-1,3-dioxolan-4yl]methoxy]phenyl]piperazine

**Supplier / Manufacturer:**

**C/D/N Isotopes Inc.**

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Website: www.cdnisotopes.com

**In case of emergency:**

**TOXYSKAN HOTLINE: 1-855-780-0599**

### Section 2. Hazards identifications

**Physical state:** Solid

**Warning:** Toxic if swallowed.

**Routes of entry:** Inhalation, ingestion, skin and eyes

#### GHS (Globally Harmonized System of Classification and Labelling of Chemicals):

**GHS Classification:**

- Acute toxicity, Oral (Category 3)
- Reproductive toxicity (Category 1B)
- Specific target organ toxicity - repeated exposure (Category 2)

**GHS Label elements:**

- Pictograms:  
- Signal word: Danger

**Hazards statement:**

- H301 Toxic if swallowed.
- H360 May damage fertility or the unborn child.
- H373 May cause damage to organs through prolonged or repeated exposure.

**Precautionary statement:**

- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
- P316 Get emergency medical help immediately.

### Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
(±)-Ketoconazole-d <sub>4</sub>	1398065-75-2	> 98

### Section 4. First aid measures

**Eye contact:** Flush eyes with water as a precaution.

**Skin contact:** Wash off with soap and plenty of water. Consult a physician.

**Inhalation:** If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**Ingestion:** Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

**General advice:** Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

## **Section 5. Firefighting measures**

**Flammability of the product:** Not flammable or combustible.

**Lower explosion limit:** No data available.

**Upper explosion limit:** No data available.

**Auto-ignition temperature:** No data available.

**Flash point:** No data available.

**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides, hydrogen chloride gas.

**Firefighting media and instructions:** Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Special protective equipment for firefighters:** Wear self-contained breathing apparatus for firefighting if necessary.

## **Section 6. Accidental release measures**

**Personal precautions:** Use personal protective equipment. Avoid dust formation. Ensure adequate ventilation. Avoid breathing dust.

**Environmental precautions:** Do not let product enter drains. Discharge into the environment must be avoided.

**Methods for cleaning up:** Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

## **Section 7. Handling and storage**

**Handling:** Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation.

**Storage:** STORE REFRIGERATED. Adequate ventilation.

## **Section 8. Exposure Controls, Personal Protections**

**Engineering controls:** Use mechanical exhaust or laboratory fumehood to avoid exposure.

**Eyes:** Safety glasses with side-shields conforming to NIOSH (US) or EN 166(EU).

**Respiratory:** Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US).

**Hands:** Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Skin/body:** Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

## **Section 9. Physical and chemical properties (unlabelled)**

**Molecular weight:** 531.43 g/mol

**Physical status:** Solid

**Color:** White to off-white

**Odour:** No data available

**Density:** No data available

**Melting point:** 146 - 147 °C (295 - 297 °F)

**Boiling point:** No data available

**Vapour pressure:** No data available

**Vapour density:** No data available

**Partition coefficient (octanol/water):** log Pow: 4.35

**Water solubility:** No data available

## **Section 10. Stability and reactivity**

**Stability and reactivity:** Stable under recommended storage conditions.

**Incompatibility:** Strong oxidizing/reducing agents.

**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen oxides, hydrogen chloride gas.

**Reactivity conditions:** No data available.

## **Section 11. Toxicological information (unlabelled)**

**Toxicological data:** (±)-Ketoconazole

### **Information on ingredients:**

<u>Name</u>	<u>CAS</u>	<u>LD<sub>50</sub></u>	<u>LC<sub>50</sub></u>
(±)-Ketoconazole	65277-42-1	Oral - Rat - 166 mg/kg	No data available

### **Potential acute effects**

- **Eyes:** May cause eye irritation.
- **Skin:** May be harmful if absorbed through skin. May cause skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** Toxic if swallowed.

### **Potential chronic effects**

- **Carcinogenic effects:** IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** Genotoxicity in vitro - Human - lymphocyte. DNA inhibition.
- **Teratogenic effects:** May damage the unborn child. Presumed human reproductive toxicant.
- **Medical conditions aggravated by overexposure:** May cause damage to organs through prolonged or repeated exposure.

## **Section 12. Ecological information**

### **Ecological data:**

<u>Name</u>	<u>Results</u>	<u>Species</u>	<u>Period</u>
(±)-Ketoconazole	No data available		

**Effects on environment:** An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

**Mobility:** No data available.

**Environmental precautions:** No data available.

**Persistence and degradability:** No data available.

**Bioaccumulative potential:** No data available.

## **Section 13. Disposal considerations**

**Waste disposal:** Contact a licensed professional waste disposal service to dispose of this material.

## **Section 14. Transportation information**

### **Classification DOT/IMDG/IATA label:**

**Shipping name:** Toxic solid, organic, n.o.s. (Ketoconazole)

**UN number:** 2811

**Class:** 6.1

**Packaging group:** III

**Additional information:** None

## **Section 15. Regulatory information**

### **UNITED STATES: NFPA classification**



Health: 3  
Flammable: 0  
Reactivity: 0  
Special conditions: None

**Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous**

### **U.S. Federal regulations:**

**TSCA 8(b) inventory:** (±)-Ketoconazole

**SARA 302/304/311/312 extremely hazardous substances:** Not Listed

**SARA 302/304 emergency planning and notification:** Not Listed

**SARA 302/304/311/312 hazardous chemicals:** Not Listed

**SARA 311/312 MSDS distribution - chemical inventory - hazard identification:** Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Not Listed

**CWA (Clean Water Act) 307:** Not Listed

**CWA (Clean Water Act) 311:** Not Listed

**CAA (Clean Air Act) 112 accidental release prevention:** Not Listed

**CAA (Clean Air Act) 112 regulated flammable substances:** Not Listed

**CAA (Clean Air Act) 112 regulated toxic substances:** Not Listed

### **State regulations:**

**DEA List I Chemicals (Precursor Chemicals):** Not Listed

**DEA List II Chemicals (Essential Chemicals):** Not Listed

**Substances in Massachusetts:** Not Listed

**Dangerous substances in New Jersey:** Not Listed

**New York – Dangerous substances with acute effects:** Not Listed

**Dangerous substances in Pennsylvania – right to know:** Not Listed

### **WHMIS (Canada):**



D1B - Toxic material causing immediate and serious toxic effects



D2A - Very toxic material causing other toxic effects

## **Section 16. Additional information**

### **References:**

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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**Elaborated by: Toxyscan Inc., 1-866-780-0599**

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