Safety Data Sheet
acc. to OSHA HCS

Date of issue: 11/18/2024 Revision date 11/18/2024

*
1 Identification

· **Product identifier**

· **Trade name: Ketoconazole-d3**
· **Synonym**
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)ethan-1-one-2,2,2-d3
· **CAS Number:**
1217766-70-5
· **Other means of identification**

· **Article number:** 10010656
· **Application of the substance / the mixture**
This product is for research use - Not for human or veterinary diagnostic or therapeutic use.

· **Details of the supplier of the safety data sheet**
· **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA

· **Information department:** Product safety department
· **Emergency telephone number:**
During normal opening times: +1 (734) 971-3335
US/CANADA: 800-424-9300
Outside US/CANADA: 703-741-5970

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2 Hazard(s) identification

· **Classification of the substance or mixture**

GHS06 Skull and crossbones

Acute toxicity - oral 3	H301 Toxic if swallowed.

GHS08 Health hazard

Reproductive toxicity 1B	H360 May damage fertility or the unborn child.
Specific target organ toxicity (repeated exposure) 2	H373 May cause damage to organs through prolonged or repeated exposure.

GHS09 Environment

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Aquatic Acute 1	H400 Very toxic to aquatic life.
Aquatic Chronic 1	H410 Very toxic to aquatic life with long lasting effects.

· **Label elements**
· **GHS label elements**
The substance is classified and labeled according to the Globally Harmonized System (GHS).
· **Hazard pictograms**

GHS06 GHS08 GHS09

· **Signal word** Danger
· **Hazard statements**
H301 Toxic if swallowed.
H360 May damage fertility or the unborn child.
H373 May cause damage to organs through prolonged or repeated exposure.
H410 Very toxic to aquatic life with long lasting effects.
· **Precautionary statements**

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P260	Do not breathe dust/fume/gas/mist/vapors/spray.
P264	Wash thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P301+P310	If swallowed: Immediately call a poison center/doctor.
P321	Specific treatment (see on this label).
P330	Rinse mouth.
P308+P313	IF exposed or concerned: Get medical advice/attention.
P314	Get medical advice/attention if you feel unwell.
P391	Collect spillage.
P405	Store locked up.
P501	Dispose of contents/container in accordance with local/regional/national/international regulations.

· **Information pertaining to particular dangers for man and environment:**
· **Classification system:**
· **NFPA ratings (scale 0 - 4)**

Health = 2
Fire = 0
Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**

Health = *2
Fire = 0
Reactivity = 0

· **Other hazards**
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable.
· **vPvB:** Not applicable.

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· **Classification according to (d)(1)(ii) of § 1910.12000**
The SDS issuer does not object to the classifications provided by importers or manufacturers of precursor products.
· **Hazards not otherwise classified**
There are no adverse physical or health effects known that are not covered by the hazard classes of the Hazard Communications Standard.

3 Composition/information on ingredients

· **Chemical characterization: Substances**
· **CAS No. Description**
1217766-70-5 Ketoconazole-d3

4 First-aid measures

· **Description of first aid measures**
· **General information:**
Immediately remove any clothing soiled by the product.
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
In case of irregular breathing or respiratory arrest provide artificial respiration.
· **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.
· **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
· **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
· **After swallowing:** Do not induce vomiting; immediately call for medical help.
· **Most important symptoms and effects, both acute and delayed**
No further relevant information available.
· **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

· **Extinguishing media**
· **Suitable extinguishing agents:**
Use fire fighting measures that suit the environment.
A solid water stream may be inefficient.
· **Special hazards arising from the substance or mixture** No further relevant information available.
· **Advice for firefighters**
· **Protective equipment:** No special measures required.

6 Accidental release measures

· **Personal precautions, protective equipment and emergency procedures** Not required.
· **Environmental precautions:**
Inform respective authorities in case of seepage into water course or sewage system.
Do not allow to enter sewers/ surface or ground water.
· **Methods and material for containment and cleaning up:**
Dispose contaminated material as waste according to section 13.
· **Protective Action Criteria for Chemicals**
· **PAC-1:** Substance is not listed.

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· **PAC-2:** Substance is not listed.
· **PAC-3:** Substance is not listed.
· **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage

· **Precautions for safe handling** Thorough dedusting.
· **Information about protection against explosions and fires:** No special measures required.

· **Conditions for safe storage, including any incompatibilities**
· **Storage:** Store in accordance with information listed on the product insert.
· **Requirements to be met by storerooms and receptacles:** No special requirements.
· **Information about storage in one common storage facility:** Not required.
· **Further information about storage conditions:** None.
· **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

· **Control parameters**
· **Components with limit values that require monitoring at the workplace:** Not required.
· **Additional information:** The lists that were valid during the creation were used as basis.

· **Exposure controls**
· **Appropriate engineering controls** No further data; see section 7.
· **Personal protective equipment:**
· **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing.
Wash hands before breaks and at the end of work.
Store protective clothing separately.
· **Breathing equipment:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
· **Protection of hands:**

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
· **Material of gloves**
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
· **Penetration time of glove material**
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

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· **Eye protection:**

Tightly sealed goggles

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9 Physical and chemical properties

· **Information on basic physical and chemical properties**	
· **General Information**	
· **Physical state**	Solid
· **Color:**	Not determined.
· **Odor:**	Characteristic
· **Structural Formula**	C26H25Cl2D3N4O4
· **Molecular Weight**	534.5 g/mol
· **Storage Buffer**	
· **Odor threshold:**	Not determined.
· **Formulation**	
· **Melting point/Melting range:**	Undetermined.
· **Boiling point/Boiling range:**	Undetermined.
· **Flammability:**	Product is not flammable.
· **Explosion limits:**	
· **Lower:**	Not determined.
· **Upper:**	Not determined.
· **Flash point:**	Not applicable.
· **Decomposition temperature:**	Not determined.
· **pH-value:**	Not applicable.
· **Viscosity:**	
· **Kinematic:**	Not applicable.
· **SOLUBILITY**	Chloroform: slightly soluble; Methanol: slightly soluble
· **Dynamic:**	Not applicable.
· **Solubility in / Miscibility with**	
· **Water:**	Not determined.
· **Partition coefficient (n-octanol/water):**	Not determined.
· **Vapor pressure:**	Not applicable.
· **Vapor pressure:**	
· **Density:**	Not determined.
· **Relative density**	Not determined.
· **Vapor density**	Not applicable.
· **Particle characteristics**	Not determined.

· **Other information**	
· **Appearance:**	
· **Form:**	Solid
· **Important information on protection of health and environment, and on safety.**	
· **Ignition temperature:**	Not determined.
· **Danger of explosion:**	Product does not present an explosion hazard.

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· **Change in condition**
· **Evaporation rate** Not applicable.

10 Stability and reactivity

· **Reactivity** No further relevant information available.
· **Chemical stability**
· **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
· **Possibility of hazardous reactions** No dangerous reactions known.
· **Conditions to avoid** No further relevant information available.
· **Incompatible materials:** strong oxidizing agents
· **Hazardous decomposition products:**
carbon dioxide, carbon monoxide, hydrogen chloride,nitrogen oxides

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11 Toxicological information

· **Information on toxicological effects**
· **Acute toxicity:**
· **Primary irritant effect:**
· **on the skin:** No irritant effect.
· **on the eye:** No irritating effect.
· **Sensitization:** No sensitizing effects known.
· **Additional toxicological information:**
· **Interactive effects** No interactive effects between components are known.

· **Carcinogenic categories**
· **IARC (International Agency for Research on Cancer)** Substance is not listed.
· **NTP (National Toxicology Program)** Substance is not listed.
· **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.
· **Alternative sources for toxicological information**
No non-standard sources for toxicological information where used.

12 Ecological information

· **Toxicity**
· **Aquatic toxicity:** No further relevant information available.
· **Persistence and degradability** No further relevant information available.
· **Bioaccumulative potential** No further relevant information available.
· **Mobility in soil** No further relevant information available.
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable.
· **vPvB:** Not applicable.
· **Other adverse effects**
· **Remark:** Very toxic for fish
· **Additional ecological information:**
· **General notes:**
Water hazard class 3 (Self-assessment): extremely hazardous for water
Do not allow product to reach ground water, water course or sewage system, even in small quantities.
Danger to drinking water if even extremely small quantities leak into the ground.

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Also poisonous for fish and plankton in water bodies.
Very toxic for aquatic organisms

13 Disposal considerations

· **Waste treatment methods**
· **Recommendation:**
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

· **Uncleaned packagings:**
· **Recommendation:** Disposal must be made according to official regulations.

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14 Transport information

· **UN-Number**	
· **DOT, IMDG, IATA**	UN2811
· **UN proper shipping name**	
· **DOT**	Toxic solids, organic, n.o.s. (Ketoconazole-d3)
· **IMDG**	TOXIC SOLID, ORGANIC, N.O.S. (Ketoconazole-d3)
· **IATA**	Toxic solid, organic, n.o.s. (Ketoconazole-d3)
· **Transport hazard class(es)**	
· **DOT**	
· **Class**	6.1 Toxic substances
· **Label**	6.1
· **IMDG**	
· **Class**	6.1 Toxic substances
· **Label**	6.1
· **IATA**	
· **Class**	6.1 Toxic substances
· **Label**	6.1
· **Packing group**	
· **DOT, IMDG, IATA**	III
· **Environmental hazards:**	Environmentally hazardous substance, solid

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· **Marine pollutant:**	Symbol (fish and tree)
· **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**	Not applicable.
· **Transport/Additional information:**	
· **DOT**	
· **Quantity limitations**	On passenger aircraft/rail: 100 kg On cargo aircraft only: 200 kg
· **IMDG**	
· **Limited quantities (LQ)**	5 kg
· **Excepted quantities (EQ)**	Code: E1 Maximum net quantity per inner packaging: 30 g Maximum net quantity per outer packaging: 1000 g
· **IATA**	
· **Remarks:**	When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.
· **Special precautions for user**	Warning: Toxic substances
· **Hazard identification number (Kemler code):**	60
· **EMS Number:**	F-A,S-A
· **Stowage Category**	A
· **UN "Model Regulation":**	UN 2811 TOXIC SOLID, ORGANIC, N.O.S. (KETOCONAZOLE-D3), 6.1, III, ENVIRONMENTALLY HAZARDOUS

15 Regulatory information

· **Safety, health and environmental regulations/legislation specific for the substance or mixture**
No further relevant information available.
· **Sara**
· **Section 355 (extremely hazardous substances):** Substance is not listed.
· **Section 313 (Specific toxic chemical listings):** Substance is not listed.
· **TSCA (Toxic Substances Control Act):** Substance is not listed.
· **Hazardous Air Pollutants** Substance is not listed.
· **Chemicals known to cause cancer:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
· **Chemicals known to cause developmental toxicity:** Substance is not listed.

· **Carcinogenic categories**
· **EPA (Environmental Protection Agency)** Substance is not listed.
· **TLV (Threshold Limit Value)** Substance is not listed.
· **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
· **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

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16 Other information

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

· **Department issuing SDS:** Environment protection department.
· **Contact:** -
· **Date of previous version** 10/03/2022
· **Date of preparation** 11/18/2024
· **Abbreviations and acronyms:**
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
PBT: Persistent, Bioaccumulative and Toxic
vPvB: very Persistent and very Bioaccumulative
NIOSH: National Institute for Occupational Safety
OSHA: Occupational Safety & Health
TLV: Threshold Limit Value
PEL: Permissible Exposure Limit
REL: Recommended Exposure Limit
Acute toxicity - oral 3: Acute toxicity – Category 3
Reproductive toxicity 1B: Reproductive toxicity – Category 1B
Specific target organ toxicity (repeated exposure) 2: Specific target organ toxicity (repeated exposure) – Category 2
Aquatic Acute 1: Hazardous to the aquatic environment - acute aquatic hazard – Category 1
Aquatic Chronic 1: Hazardous to the aquatic environment - long-term aquatic hazard – Category 1
· *** Data compared to the previous version altered.**