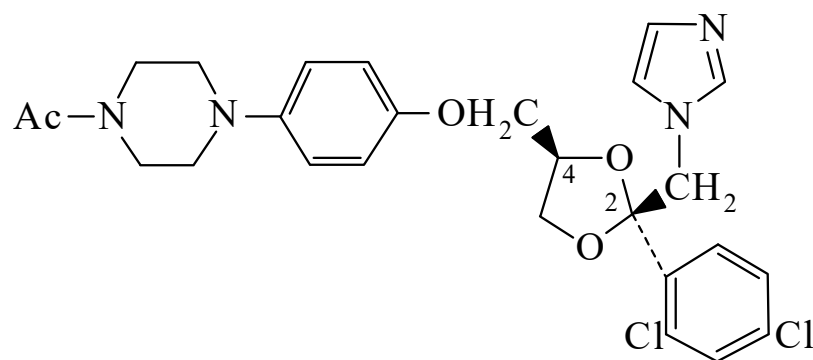




>>Entry Name: Ketoconazole, BAN, INN, JAN, USAN

Synonym(s): 1-Acetyl-4-[4-[[2-(2,4-dichlorophenyl)-2-(1*H*-imidazol-1-yl)methyl]-1,3-dioxolan-4-yl]methoxy]phenyl]piperazine, 9Cl. Fungarest. Fungoral. Ketoderm. Nizoral. Terzolin. Triatop. R 41400. Many other names



Molecular Formula: C₂₆H₂₈Cl₂N₄O₄

Molecular Weight: 531.437

Accurate Mass: 530.14876

Percentage Composition: C 58.76%; H 5.31%; Cl 13.34%; N 10.54%; O 12.04%

Biological Use/Importance: Functions as Lanosterol C-14 demethylation inhibitor. Antifungal agent

Development Status: Marketed drug

Calculated Log P Data: Log P 4.74 (calc)

Hazard & Toxicity: Adverse effects incl. gastrointestinal disturbances, hepatotoxicity, and effects on endocrine system. LD₅₀ (rat, orl) 166 mg/kg. Exp. reprod. effects

>>Variant: (2*RS*,4*RS*)-form

Synonym(s): (±)-*cis*-form

CAS Registry Number: 65277-42-1

Molecular Formula: C₂₆H₂₈Cl₂N₄O₄

Molecular Weight: 531.437

Accurate Mass: 530.14876

Percentage Composition: C 58.76%; H 5.31%; Cl 13.34%; N 10.54%; O 12.04%

Physical Description: Cryst. (4-methyl-2-pentanone)

Melting Point: Mp 146°

Other Data: Orally active but activity limited by bioavailability

Sigma: K1003

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