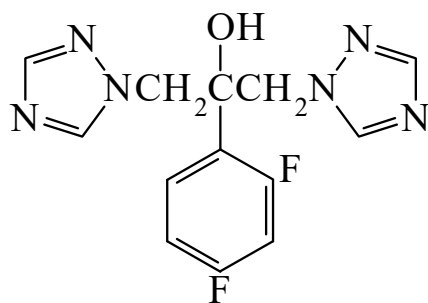




>>Entry Name: Fluconazole, BAN, INN, JAN, USAN

Synonym(s): α -(2,4-Difluorophenyl)- α -(1*H*-1,2,4-triazol-1-ylmethyl)-1*H*-1,2,4-triazole-1-ethanol, 9Cl. 2-(2,4-Difluorophenyl)-1,3-bis(1*H*-1,2,4-triazol-1-yl)-2-propanol. Biozolen. Diflucan. Elazor. Fungata. Triflucan. UK 49858. Many other names



CAS Registry Number: 86386-73-4

Related CAS Registry Numbers(s): 123631-92-5

Molecular Formula: C₁₃H₁₂F₂N₆O

Molecular Weight: 306.274

Accurate Mass: 306.104065

Percentage Composition: C 50.98%; H 3.95%; F 12.41%; N 27.44%; O 5.22%

Biological Use/Importance: Antifungal agent. Effective in single oral dose against vaginal candidiasis. Prophylactic treatment for AIDS patients. Not active against *Aspergillus*

Physical Description: Cryst. (EtOAc/hexane)

Development Status: Marketed drug. Launched 1988. Worldwide 42nd best selling prescription drug (\$1.01 bn) (Pfizer) (2000, Pharma Business)

Melting Point: Mp 138-140°

Calculated Log P Data: Log P -0.11 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 1271 mg/kg

>>Derivative: Dihydrogen phosphate ester

Synonym(s): Fosfluconazole, BAN, INN. UK 292 663

CAS Registry Number: 194798-83-9

Molecular Formula: C₁₃H₁₃F₂N₆O₄P

Molecular Weight: 386.254

Accurate Mass: 386.070397

Percentage Composition: C 40.42%; H 3.39%; F 9.84%; N 21.76%; O 16.57%; P 8.02%

Biological Use/Importance: Antifungal agent

Physical Description: Solid

Melting Point: Mp 223-224°

>>Derivative: Dihydrogen phosphate ester, di-Na salt

CAS Registry Number: 194798-85-1

Physical Description: Solid

Melting Point: Mp 160-162°

References:

- U.K. Pat., 1982, Pfizer, 2 099 818; CA, **99**, 38467q, (synth, pharmacol)
Grant, S.M. *et al.*, *Drugs*, 1990, **39**, 877, (rev)
Cobos Garcia, F.J. *et al.*, *Farm. Clin.*, 1991, **8**, 423, (rev)
Morck, H., *Pharm. Ztg.*, 1991, **136**, 56; 60, (rev)
Morita, K. *et al.*, *Chem. Pharm. Bull.*, 1992, **40**, 1247, (pharmacol)
Fluconazole, (Eds., Powderly, W.G. *et al.*), Marius Press, 1992, (book)
Urbak, S.F. *et al.*, *Ophthalmologica*, 1994, **208**, 147, (use, rev)
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 7th edn., Akademie-Verlag, 1994, 3349, (synonyms)
Goa, K.L. *et al.*, *Drugs*, 1995, **50**, 658, (rev, pharmacokinetic)
Pat. Coop. Treaty (WIPO), 1997, Pfizer, 97 28 169; CA, **127**, 220800s, (fosfluconazole, synth, pharmacol)
Martindale, *The Extra Pharmacopoeia*, 32nd edn., Pharmaceutical Press, 1999, 378