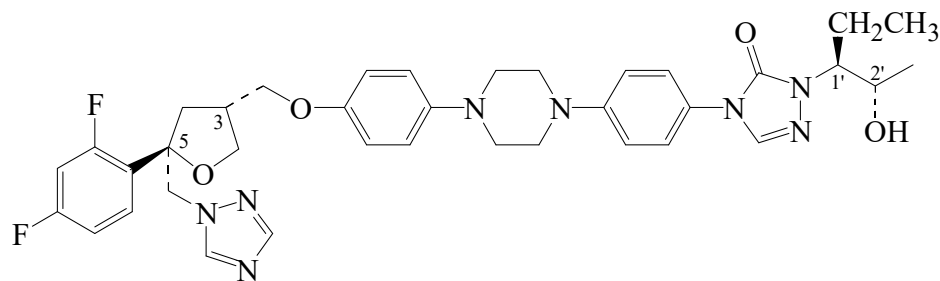




>>Entry Name: Posaconazole, INN, USAN

Synonym(s): 4-[4-[4-[4-[[5-(2,4-Difluorophenyl)tetrahydro-5-(1*H*-1,2,4-triazol-1-ylmethyl)-3-furanyl]methoxy]phenyl]-1-piperazinyl]phenyl]-2-(1-ethyl-2-hydroxypropyl)-2,4-dihydro-3*H*-1,2,4-triazol-3-one, 9Cl. Sch 56592



CAS Registry Number: 171228-49-2

Extra CAS Registry Numbers(s): 170985-61-2 171228-50-5 171228-51-6

Molecular Formula: C₃₇H₄₂F₂N₈O₄

Molecular Weight: 700.787

Accurate Mass: 700.329708

Percentage Composition: C 63.42%; H 6.04%; F 5.42%; N 15.99%; O 9.13%

Biological Use/Importance: Broad spectrum orally active antifungal agent

Melting Point: Mp 164-165°

Optical Rotation: $[\alpha]_D^{25} -29$ (c, 1 in CHCl₃)

Other Data: Stereochem. is (1'S,2'S,3R,5R)

References:

- Pat. Coop. Treaty (WIPO)*, 1995, *Schering*, 95 17 407; *CA*, **124**, 8599b, (*synth, pharmacol*)
Sugar, A.M. *et al.*, *Antimicrob. Agents Chemother.*, 1996, **40**, 1314-1316, (*pharmacol*)
Perfect, J.R. *et al.*, *Antimicrob. Agents Chemother.*, 1996, **40**, 1910-1913, (*pharmacol*)
Saksena, A.K. *et al.*, *Tet. Lett.*, 1996, **37**, 5657-5660, (*synth, intermed*)
Oakley, K.L., *Antimicrob. Agents Chemother.*, 1997, **41**, 1124-1126; 1504-1507, (*activity*)
Lutz, J.E. *et al.*, *Antimicrob. Agents Chemother.*, 1997, **41**, 1558-1561, (*activity*)