AZACONAZOLE

Other names: 1H-1,2,4-Triazole, 1-[[2-(2,4-dichlorophenyl)-1,3-dioxolan-2-yl]methyl]-
1-[[2-(2,4-Dichlorophenyl)-1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole
Azoconazole
R-28644

Inchi: InChI=1S/C12H11Cl2N3O2/c13-10-3-9(4-11(14)5-10)12(18-1-2-19-12)6-17-8-15-7-16-17

InchiKey: ULXPFHRWKJWAAE-UHFFFAOYSA-N

Formula: C12H11Cl2N3O2

SMILES: Clc1cc(Cl)cc(C2(Cn3cncn3)OCCO2)c1

Mol. weight [g/mol]: 300.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Cheméo Relay (1.0)
logp	2.485		Crippen Method
mcvol	192.020	ml/mol	McGowan Method
rinpol	2216.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60207310&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices