Miconazole

Other names: 1-[2,4-Dichloro-«beta»-[(2,4-dichlorobenzyl)oxy]phenethyl]imidazole
1-[2,4-Dichloro-Â«betaÂ»-[(2,4-dichlorobenzyl)oxy]phenethyl]imidazole
1-[2-(2,4-dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]imidazole
1H-Imidazole, 1-[2-(2,4-dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]-
Daktarin IV
Imidazole, 1-(2,4-dichloro-«beta»-((2,4-dichlorobenzyl)oxy)phenethyl)-
Imidazole, 1-(2,4-dichloro-Â«betaÂ»-((2,4-dichlorobenzyl)oxy)phenethyl)-
Imidazole, 1-(2-(2,4-dichlorophenyl)-2-((2,4-dichlorophenyl)methoxy)ethyl)-
MJR 1762
Minostate
Monistat
Monistat IV
NSC 170986
R 18134

Inchi: InChI=1S/C18H14Cl4N2O/c19-13-2-1-12(16(21)7-13)10-25-18(9-24-6-5-23-11-24)15-4-3

InchiKey: BYBLEWFAAKGYCD-UHFFFAOYSA-N

Formula: C18H14Cl4N2O

SMILES: Clc1ccc(COC(Cn2ccnc2)c2ccc(Cl)cc2Cl)c(Cl)c1

Mol. weight [g/mol]: 416.13

CAS: 22916-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Aqueous Solubility Prediction Method
logp	6.455		Crippen Method
mcvol	272.290	ml/mol	McGowan Method
rinpol	2962.00		NIST Webbook
rinpol	2980.00		NIST Webbook
rinpol	2980.00		NIST Webbook
rinpol	2980.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22916478&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices