ketoconazole

Other names:	1-[4-(4-{[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]meth
Inchi:	InChI=1S/C26H28Cl2N4O4/c1-19(33)31-10-12-32(13-11-31)21-3-5-22(6-4-21)34-15-23-1
InchiKey:	XMAYWYJOQHXEEK-OZXSUGGESA-N
Formula:	C26H28Cl2N4O4
SMILES:	CC(=O)N1CCN(c2ccc(OCC3COC(Cn4ccnc4)(c4ccc(Cl)cc4Cl)O3)cc2)CC1
Mol. weight [g/mol]:	531.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Cheméo Relay (1.0)
logp	4.206		Crippen Method
mcvol	372.080	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Measurement and correlation of antifungal drugs solubility in pure supercritical CO2 using semiempirical models:	https://www.doi.org/10.1016/j.jct.2011.02.020
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

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