Fluquiconazole

Inchi: InChI=1S/C13H12F2N6O/c14-11-3-10(4-12(15)5-11)13(22,6-20-9-16-8-19-20)7-21-17-1-
InchiKey: CZWLHKHODFNZFU-UHFFFAOYSA-N
Formula: C13H12F2N6O
SMILES: OC(Cn1cncn1)(Cn1nccn1)c1cc(F)cc(F)c1
Mol. weight [g/mol]: 306.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	0.736		Crippen Method
mcvol	200.640	ml/mol	McGowan Method
rinpol	2723.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R194908&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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