

CYPROCONAZOLE

Other names: Cyproconazole, isomer 2
Inchi: InChI=1S/C15H18ClN3O/c1-11(12-2-3-12)15(20,8-19-10-17-9-18-19)13-4-6-14(16)7-5-1
InchiKey: UFNOKDBUJZYDE-UHFFFAOYSA-N
Formula: C15H18ClN3O
SMILES: CC(C1CC1)C(O)(Cn1cncn1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 291.78
CAS: 113096-99-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	2.865		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
rinpol	2238.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2238.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C113096994&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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