

propiconazole-1

Other names: Propiconazole I
Inchi: InChI=1S/C15H17Cl2N3O2/c1-2-3-12-7-21-15(22-12,8-20-10-18-9-19-20)13-5-4-11(16)6
InchiKey: STJLVHWMYQXCPB-UHFFFAOYSA-N
Formula: C15H17Cl2N3O2
SMILES: CCCC1COC(Cn2cn2)(c2ccc(Cl)cc2Cl)O1
Mol. weight [g/mol]: 342.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	3.653		Crippen Method
mcvol	234.290	ml/mol	McGowan Method
rinpol	2333.00		NIST Webbook
rinpol	2342.00		NIST Webbook
rinpol	2333.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R396991&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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