

difenoconazole-2

Other names:	Difenoconazole, isomer 2
Inchi:	InChI=1S/C19H17Cl2N3O3/c1-13-9-25-19(27-13,10-24-12-22-11-23-24)17-7-6-16(8-18)
InchiKey:	BQYJATMQXGBDHF-UHFFFAOYSA-N
Formula:	C19H17Cl2N3O3
SMILES:	CC1COC(Cn2cncn2)(c2ccc(Oc3ccc(Cl)cc3)cc2Cl)O1
Mol. weight [g/mol]:	406.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Crippen Method
logp	4.665		Crippen Method
mcvol	272.760	ml/mol	McGowan Method
rinpol	3025.00		NIST Webbook
rinpol	3027.00		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=R404101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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