

Difenoconazole

Other names:	Difenconazole Bardos Neu CGA 169374 Score EC 250 Dragon Plover Dividend Score 1H-1,2,4-Triazole, 1-((2-(2-chloro-4-(4-chlorophenoxy)phenyl)-4-methyl-1,3-dioxolan-2-yl)methyl)- difenaconazole 1-[2-[2-chloro-4-(4-chlorophenoxy)phenyl]-4-methyl-1,3-dioxolan-2-ylmethyl]-1H-1,2,4-tria
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
CAS:	119446-68-3

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	3136.00		NIST Webbook
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rinpol	3136.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119446683&Units=SI

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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