

Vinclozoline

Other names:	2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- 2,4-Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-methyl-5-vinyl- 3-(3,5-Dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione 3-(3,5-Dichlorophenyl)-5-methyl-5-vinyl-1,3-oxazolidin-2,4-dion 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl-1,3-oxazolidine-2,4-dione BAS 352 F BAS 35204F Mascot contact turf fungicide N-3,5-Dichlorophenyl-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione Ornalin Oxazolidinedione, 3-(3,5-dichlorophenyl)-5-ethenyl-5-methyl- Ronilan Ronilan 50WP Ronilon Vinclozalin Vinclozlin Vinclozolin Vorlan
Inchi:	InChI=1S/C12H9Cl2NO3/c1-3-12(2)10(16)15(11(17)18-12)9-5-7(13)4-8(14)6-9/h3-6H,1H
InchiKey:	FSCWZHGZWDELK-UHFFFAOYSA-N
Formula:	C12H9Cl2NO3
SMILES:	C=CC1(C)OC(=O)N(c2cc(Cl)cc(Cl)c2)C1=O
Mol. weight [g/mol]:	286.11
CAS:	50471-44-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Estimated Solubility Method
log10ws	-4.93		Aqueous Solubility Prediction Method
logp	3.421		Crippen Method
mcvol	184.490	ml/mol	McGowan Method
rinpol	1889.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1883.00		NIST Webbook

rinpol	1877.00		NIST Webbook
rinpol	1858.00		NIST Webbook
rinpol	1844.00		NIST Webbook
ripol	2744.00		NIST Webbook
ripol	2744.00		NIST Webbook
tf	383.69 ± 0.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50471448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
ripol:	Polar retention indices
tf:	Normal melting (fusion) point

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