

Fluquinconazole

Other names:	3-(2,4-Dichlorophenyl)-6-fluoro-2-(1H-1,2,4-triazol-1-yl)quinazolin-4(3H)-one 3-(2,4-Dichlorophenyl)-6-fluoro-2-(1H-1,2,4-triazol-1-yl)-4(3H)-quinazolinone 4(3H)-Quinazolinone, 3-(2,4-dichlorophenyl)-6-fluoro-2-(1H-1,2,4-triazol-1-yl)-
Inchi:	InChI=1S/C16H8Cl2FN5O/c17-9-1-4-14(12(18)5-9)24-15(25)11-6-10(19)2-3-13(11)22-16
InchiKey:	IJJVMEJXYNJXOJ-UHFFFAOYSA-N
Formula:	C16H8Cl2FN5O
SMILES:	O=c1c2cc(F)ccc2nc(-n2cncn2)n1-c1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	376.17
CAS:	136426-54-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.00		Crippen Method
logp	3.412		Crippen Method
mcvol	231.880	ml/mol	McGowan Method
rinpol	2729.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C136426545&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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