

QUINOXYFEN

Other names:	Quinoline, 5,7-dichloro-4-(4-fluorophenoxy)- 5,7-dichloro-4-(4-fluorophenoxy)quinoline
Inchi:	InChI=1S/C15H8Cl2FNO/c16-9-7-12(17)15-13(8-9)19-6-5-14(15)20-11-3-1-10(18)2-4-11
InchiKey:	WRPIRSINYZBGPK-UHFFFAOYSA-N
Formula:	C15H8Cl2FNO
SMILES:	Fc1ccc(Oc2ccnc3cc(Cl)cc(Cl)c23)cc1
Mol. weight [g/mol]:	308.13
CAS:	124495-18-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.38		Crippen Method
logp	5.473		Crippen Method
mcvol	197.330	ml/mol	McGowan Method
rinpol	2347.00		NIST Webbook
rinpol	2353.00		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=C124495187&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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