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