Pyriproxyfen

Other names:	Pyridine, 2-[1-methyl-2-(4-phenoxyphenoxy)ethoxy]- pyriproxifen 2-[1-methyl-2-(4-phenoxyphenoxy)ethoxy]pyridine
Inchi:	InChI=1S/C20H19NO3/c1-16(23-20-9-5-6-14-21-20)15-22-17-10-12-19(13-11-17)24-18-7
InchiKey:	NHDHVHZZCFYRSB-UHFFFAOYSA-N
Formula:	C20H19NO3
SMILES:	CC(COc1ccc(Oc2ccccc2)cc1)Oc1ccccn1
Mol. weight [g/mol]:	321.37
CAS:	95737-68-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	4.720		Crippen Method
mcvol	248.970	ml/mol	McGowan Method
rinpol	2574.00		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=C95737681&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