Diphenylpyraline

Other names:	Piperidine, 4-(diphenylmethoxy)-1-methyl-
	AN 1041
	Belfene
	Dayfen
	Diphenylpyrilene
	Hispril
	Histryl
	Histyn
	Hystryl
	Lyssipoll
	Mepiben
	N-Methyl-4-(Benzhydryloxy)piperidine
	Neargal
	P 253
	1-Methyl-4-Piperidyl benzhydryl ether
	4-(Benzhydryloxy)-1-methylpiperidine
	Allergen
	4-(Diphenylmethoxy)-1-methylpiperidine
	N-Methylpiperidyl-(4)-benzhydrylaether salzsauren salze
	Diphenylpyralamine
Inchi:	InChI=1S/C19H23NO/c1-20-14-12-18(13-15-20)21-19(16-8-4-2-5-9-16)17-10-6-3-7-11-1
InchiKey:	OWQUZNMMYNAXSL-UHFFFAOYSA-N
Formula:	C19H23NO
SMILES:	CN1CCC(OC(c2ccccc2)c2ccccc2)CC1
Mol. weight [g/mol]:	281.39
CAS:	147-20-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.21		Crippen Method
logp	3.887		Crippen Method
mcvol	236.040	ml/mol	McGowan Method
rinpol	2101.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2099.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2101.00		NIST Webbook

rinpol	2100.00	NIST Webbook
rinpol	2099.00	NIST Webbook
rinpol	2099.00	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=C147206&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