Oxypertine

Other names:	1H-Indole, 5,6-dimethoxy-2-methyl-3-[2-(4-phenyl-1-piperazinyl)ethyl]- Indole, 5,6-dimethoxy-2-methyl-3-(2-(4-phenyl-1-piperazinyl)ethyl)- Equipertine Forit Integrin Opertil Oxypertin WIN 18501-2 5,6-Dimethoxy-2-methyl-3-[2-(4-phenyl-1-piperazinyl)ethyl]indole Oxipertine
Inchi:	InChI=1S/C23H29N3O2/c1-17-19(20-15-22(27-2)23(28-3)16-21(20)24-17)9-10-25-11-13
InchiKey:	XCWPUUGSGHNIDZ-UHFFFAOYSA-N
Formula:	C23H29N3O2
SMILES:	COc1cc2[nH]c(C)c(CCN3CCN(c4ccccc4)CC3)c2cc1OC
Mol. weight [g/mol]:	379.50
CAS:	153-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	3.376		Crippen Method
mcvol	303.070	ml/mol	McGowan Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook

Sources

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=C153877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices