Piminodine

Other names:	4-Piperidinecarboxylic acid, 4-phenyl-1-[3-(phenylamino)propyl]-, ethyl ester
	Isonipecotic acid, 1-(3-anilinopropyl)-4-phenyl-, ethyl ester
	Alvodine
	Anopridine
	Cimadon
	NIH 7590
	Pimadin
	Pimadine
	WIN 14098
	4-Phenyl-1-(3-(phenylamino)propyl)-4-piperidinecarboxylic acid ethyl ester
	WIN 14098-2
	Pimadin (analgesic)
Inchi:	InChI=1S/C23H30N2O2/c1-2-27-22(26)23(20-10-5-3-6-11-20)14-18-25(19-15-23)17-9-16
InchiKey:	PXXKIYPSXYFATG-UHFFFAOYSA-N
Formula:	C23H30N2O2
SMILES:	CCOC(=O)C1(c2ccccc2)CCN(CCCNc2ccccc2)CC1
Mol. weight [g/mol]:	366.50
CAS:	13495-09-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	4.086		Crippen Method
mcvol	303.950	ml/mol	McGowan Method
rinpol	2885.00		NIST Webbook
rinpol	2891.00		NIST Webbook
rinpol	2885.00		NIST Webbook
rinpol	2891.00		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

Legend

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