Pipamperone

Other names:	(1,4'-Bipiperidine)-4'-carboxamide, 1'-(3-(p-fluorobenzoyl)propyl)-
	Dipiperal
	Dipiperon
	Dipiperone
	Floropipamide
	1'-(3-(p-Fluorobenzoyl)propyl)(1,4'-bipiperidine)-4'-carboxamide
	4'-Fluoro-4-(4-N-piperidino-4-carbamidopiperidino)butyrophenone
	p-Fluoro-«gamma»-(4-piperidino-4-carbamoylpiperidino)butyrophenone
	Isonipecotamide, 1-(3-(p-fluorobenzoyl)propyl)-4-piperidino-
	McN-JR-3345
	Pipaneperone
	Piperonyl
	R 3345
	[1,4'-Bipiperidine]-4'-carboxamide, 1'-[4-(4-fluorophenyl)-4-oxobutyl]-
Inchi:	InChI=1S/C21H30FN3O2/c22-18-8-6-17(7-9-18)19(26)5-4-12-24-15-10-21(11-16-24,20(2
InchiKey:	AXKPFOAXAHJUAG-UHFFFAOYSA-N
Formula:	C21H30FN3O2
SMILES:	NC(=O)C1(N2CCCCC2)CCN(CCCC(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	375.48
CAS:	1893-33-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	2.594		Crippen Method
mcvol	296.120	ml/mol	McGowan Method
rinpol	3090.00		NIST Webbook
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
rinpol	3090.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1893330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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