

Spiperone

Other names:	1,3,8-Triazaspiro[4.5]decan-4-one, 8-[4-(4-fluorophenyl)-4-oxobutyl]-1-phenyl- 1,3,8-Triazaspiro[4.5]decan-4-one, 8-[3-(p-fluorobenzoyl)propyl]-1-phenyl- R 5147 Spiroperidol Spiropitan E 525 8-(3-(p-Fluorobenzoyl)propyl)-1-phenyl-1,3,8-triazaspiro(4.5)decan-4-one Butyrophenone, 4'-fluoro-4-(4-oxo-1-phenyl-1,3,8-triazaspiro(4,5)decan-8-yl)- 8-(3-p-Fluorobenzoyl-1-propyl)-4-oxo-1-phenyl-1,3,8-triazaspiro(4,5)decane NSC 170983 Spiroperidone
Inchi:	InChI=1S/C23H26FN3O2/c24-19-10-8-18(9-11-19)21(28)7-4-14-26-15-12-23(13-16-26)2
InchiKey:	DKGZKTPJOSAWFA-UHFFFAOYSA-N
Formula:	C23H26FN3O2
SMILES:	O=C(CCCN1CCC2(CC1)C(O)=NCN2c1ccccc1)c1ccc(F)cc1
Mol. weight [g/mol]:	395.47
CAS:	749-02-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	4.057		Crippen Method
mcvol	300.540	ml/mol	McGowan Method
rinpol	3316.00		NIST Webbook
rinpol	3316.00		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=C749020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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