

Fluspirilene

Other names:	1,3,8-Triazaspiro[4.5]decan-4-one, 8-[4,4-bis(4-fluorophenyl)butyl]-1-phenyl-1,3,8-Triazaspiro[4.5]decan-4-one, 8-[4,4-bis(p-fluorophenyl)butyl]-1-phenyl-Fluspirilene Imap McN-JR 6218 R 6218 8-(4,4-Bis(p-fluorophenyl)butyl)-1-phenyl-1,3,8-triazaspiro(4,5)decan-4-one 1-Phenyl-4-oxo-8-(4,4-bis(4-fluorophenyl)butyl)-1,3,8-triazaspiro(4,5)decane Redeptin
Inchi:	InChI=1S/C29H31F2N3O/c30-24-12-8-22(9-13-24)27(23-10-14-25(31)15-11-23)7-4-18-3
InchiKey:	QOYHHIBFXOOADH-UHFFFAOYSA-N
Formula:	C29H31F2N3O
SMILES:	O=C1NCN(c2ccccc2)C12CCN(CCCC(c1ccc(F)cc1)c1ccc(F)cc1)CC2
Mol. weight [g/mol]:	475.57
CAS:	1841-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.04		Crippen Method
logp	5.305		Crippen Method
mcvol	361.520	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1841196&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

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