Cyproheptadine

Other names:	1-Methyl-4-(5H-dibenzo[a,d]cycloheptenylidene)piperidine
	4-(5H-Dibenzo(a,d)cyclohepten-5-ylidene)-1-methylpiperidine
	Cypoheptadine
	Cyproheptadiene
	Dronactin
	Eiproheptadine
	MK 141
	Periactin
	Periactine
	Periactinol
	Piperidine, 4-(5H-dibenzo[a,d]cyclohepten-5-ylidene)-1-methyl-
Inchi:	InChI=1S/C21H21N/c1-22-14-12-18(13-15-22)21-19-8-4-2-6-16(19)10-11-17-7-3-5-9-20(
InchiKey:	JJCFRYNCJDLXIK-UHFFFAOYSA-N
Formula:	C21H21N
SMILES:	CN1CCC(=C2c3ccccc3C=Cc3ccccc32)CC1
Mol. weight [g/mol]:	287.40
CAS:	129-03-3

Physical Properties

Property code	Value	Unit	Source
ie	7.94 ± 0.06	eV	NIST Webbook
log10ws	-3.09		Aqueous Solubility Prediction Method
log10ws	-1.90		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	4.698		Crippen Method
mcvol	238.890	ml/mol	McGowan Method
rinpol	2400.00		NIST Webbook
rinpol	2356.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2366.00		NIST Webbook
rinpol	2366.00		NIST Webbook

rinpol	2366.00		NIST Webbook
tf	385.52	K	Aqueous Solubility Prediction Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C129033&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point