Clothiapine

Other names:	Dibenzo[b,f][1,4]thiazepine, 2-chloro-11-(4-methyl-1-piperazinyl)-
	2-Chloro-11-(4-methylpiperazino)dibenzo(b,f)(1,4)thiazepine
	2-Chloro-11-(4-methyl-1-piperazinyl)dibenzo(b,f)(1,4)thiazepine
	Clotiapine
	Entumin
	Etumine
	HF 2159
	LW 2159
	S-805C
	Entumine
Inchi:	InChI=1S/C18H18ClN3S/c1-21-8-10-22(11-9-21)18-14-12-13(19)6-7-16(14)23-17-5-3-2-4
InchiKey:	KAAZGXDPUNNEFN-UHFFFAOYSA-N
Formula:	C18H18ClN3S
SMILES:	CN1CCN(C2=Nc3ccccc3Sc3ccc(Cl)cc32)CC1
Mol. weight [g/mol]:	343.87
CAS:	2058-52-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	4.130		Crippen Method
mcvol	249.470	ml/mol	McGowan Method
rinpol	2710.00		NIST Webbook
rinpol	2683.00		NIST Webbook
rinpol	2705.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2058528&Units=SI
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