Clozapine

Other names:	5H-Dibenzo[b,e][1,4]diazepine, 8-chloro-11-(4-methyl-1-piperazinyl)-
	8-Chloro-11-(4-methyl-1-piperazinyl)-5H-dibenzo(b,e)(1,4)diazepine
	8-Chloro-11-(4-methyl-1-piperazinyl)-5H-dibenzo[b,e] [1,4]diazepine (clozapine)
	Asaleptin
	Azaleptine
	Clozapin
	Clozaril
	Fazaclo
	HF-1854
	Iprox
	Leponex
	Lepotex
	W-801
Inchi:	InChI=1S/C18H19ClN4/c1-22-8-10-23(11-9-22)18-14-4-2-3-5-15(14)20-16-7-6-13(19)12-
InchiKey:	QZUDBNBUXVUHMW-UHFFFAOYSA-N
Formula:	C18H19ClN4
SMILES:	CN1CCN(C2=Nc3cc(Cl)ccc3Nc3ccccc32)CC1
Mol. weight [g/mol]:	326.82
CAS:	5786-21-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Aqueous Solubility Prediction Method
logp	3.723		Crippen Method
mcvol	243.100	ml/mol	McGowan Method
rinpol	2859.00		NIST Webbook
rinpol	3093.20		NIST Webbook
rinpol	2893.00		NIST Webbook
rinpol	2873.00		NIST Webbook
rinpol	2915.00		NIST Webbook
rinpol	2893.00		NIST Webbook
rinpol	2859.00		NIST Webbook
rinpol	3093.20		NIST Webbook
tf	456.78	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	35.90	kJ/mol	457.10	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5786210&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

Legend

hfust: Enthalpy of fusion at a given temperature

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