Trazodone

Other names:	1,2,4-Triazolo[4,3-a]pyridin-3(2H)-one, 2-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]-
	25332-39-2 (hydrochloride)
	Desyrel
	Trazodon
	s-Triazolo(4,3-a)pyridin-3(2H)-one, 2-(3-(4-(m-chlorophenyl)-1-piperazinyl)propyl)-
Inchi:	InChI=1S/C19H22ClN5O/c20-16-5-3-6-17(15-16)23-13-11-22(12-14-23)8-4-10-25-19(26)
InchiKey:	PHLBKPHSAVXXEF-UHFFFAOYSA-N
Formula:	C19H22ClN5O
SMILES:	O=c1n(CCCN2CCN(c3cccc(Cl)c3)CC2)nc2ccccn12
Mol. weight [g/mol]:	371.86
CAS:	19794-93-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Aqueous Solubility Prediction Method
logp	2.362		Crippen Method
mcvol	273.040	ml/mol	McGowan Method
rinpol	3345.00		NIST Webbook
rinpol	3345.00		NIST Webbook
rinpol	3300.00		NIST Webbook
rinpol	3300.00		NIST Webbook
rinpol	3345.00		NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19794935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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