Olanzapine

Other names:	Zyprexa
	10H-Thieno[2,3-b][1,5]benzodiazepine, 2-methyl-4-(4-methyl-1-piperazinyl)-
Inchi:	InChI=1S/C17H20N4S/c1-12-11-13-16(21-9-7-20(2)8-10-21)18-14-5-3-4-6-15(14)19-17(1
InchiKey:	KVWDHTXUZHCGIO-UHFFFAOYSA-N
Formula:	C17H20N4S
SMILES:	Cc1cc2c(s1)Nc1ccccc1N=C2N1CCN(C)CC1
Mol. weight [g/mol]:	312.43
CAS:	132539-06-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	3.439		Crippen Method
mcvol	237.420	ml/mol	McGowan Method
rinpol	2844.10		NIST Webbook
rinpol	2844.10		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C132539061&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
rinpol:	Non-polar retention indices