N-Desmethyl mianserin

Other names:	Desmethylmianserin
	Normianserine
	Dibenzo[c,f]pyrazino[1,2-a]azepine, 1,2,3,4,10,14b-hexahydro-
	(±)-1,2,3,4,10,14b-Hexahydro-dibenzo[c,f]pyrazino[1,2-a]azepine
Inchi:	InChI=1S/C17H18N2/c1-3-7-15-13(5-1)11-14-6-2-4-8-16(14)19-10-9-18-12-17(15)19/h1-
InchiKey:	ZBILSSSEXRZGKS-UHFFFAOYSA-N
Formula:	C17H18N2
SMILES:	c1ccc2c(c1)Cc1ccccc1N1CCNCC21
Mol. weight [g/mol]:	250.34
CAS:	71936-92-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	2.742		Crippen Method
mcvol	201.110	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71936920&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

Latest version available from: