

Mirtazapine

Other names:	Pyrazino[2,1-a]pyrido[2,3-c][2]benzazepine, 1,2,3,4,10,14b-hexahydro-2-methyl-, (+/-)- Pyrazino[2,1-a]pyrido[2,3-c][2]benzazepine, 1,2,3,4,10,14b-hexahydro-2-methyl- 1,2,3,4,10,14b-Hexahydro-2-methylpyrazino[2,1-a]pyrido[2,3-c](2)benzazepine 6-Azamianserin Mepirzepine Mirtazepine Org 3770 Remeron 2-Methyl-1,2,3,4,10,14b-hexahydropyrazino[2,1-a]pyrido[2,3-c][2]benzazepine Avanza Mepirzapin Mirtazipine Norset Promyrtil Remergil Remergon Remeron SolTab Rexer Zispin (±)-1,2,3,4,10,14b-hexahydro-2-methylpyrazino[2,1-a]pyrido[2,3-c][2]benzazepine
Inchi:	InChI=1S/C17H19N3/c1-19-9-10-20-16(12-19)15-7-3-2-5-13(15)11-14-6-4-8-18-17(14)20
InchiKey:	RONZAEMNMFQXRA-UHFFFAOYSA-N
Formula:	C17H19N3
SMILES:	CN1CCN2c3ncccc3Cc3ccccc3C2C1
Mol. weight [g/mol]:	265.35
CAS:	85650-52-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.479		Crippen Method
mcvol	211.090	ml/mol	McGowan Method
rinpol	2323.40		NIST Webbook
rinpol	2323.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C85650528&Units=SI

Legend

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

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