

Mianserin

Other names:

Dibenzo[c,f]pyrazino[1,2-a]azepine, 1,2,3,4,10,14b-hexahydro-2-methyl-1,2,3,4,10,14b-Hexahydro-2-methyldibenzo(c,f)pyrazino(1,2-a)azepine

Mianserine

Mianseryna

Inchi: InChI=1S/C18H20N2/c1-19-10-11-20-17-9-5-3-7-15(17)12-14-6-2-4-8-16(14)18(20)13-19

InchiKey: UEQUQVLFIP OEMF-UHFFFAOYSA-N

Formula: C18H20N2

SMILES: CN1CCN2c3ccccc3Cc3ccccc3C2C1

Mol. weight [g/mol]: 264.36

CAS: 24219-97-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	3.084		Crippen Method
mcvol	215.200	ml/mol	McGowan Method
rinpol	2207.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2207.00		NIST Webbook

Sources

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

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=C24219974&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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