

Mirtazapine-M (nor-) AC

Inchi: InChI=1S/C18H19N3O/c1-13(22)20-9-10-21-17(12-20)16-7-3-2-5-14(16)11-15-6-4-8-19-
InchiKey: CJOYCNYGNJLOOW-UHFFFAOYSA-N
Formula: C18H19N3O
SMILES: CC(=O)N1CCN2c3ncccc3Cc3ccccc3C2C1
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.396		Crippen Method
mcvol	226.750	ml/mol	McGowan Method
rinpol	2700.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R331063&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

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<https://www.chemeo.com/cid/24-747-6/Mirtazapine-M-nor-AC.pdf>

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