

Mirtazapine-M (nor-HO-) 2AC

Inchi: InChI=1S/C20H21N3O3/c1-13(24)22-8-9-23-19(12-22)18-6-5-17(26-14(2)25)11-16(18)10
InchiKey: QTLVDFCJBXBTJP-UHFFFAOYSA-N
Formula: C20H21N3O3
SMILES: CC(=O)Oc1ccc2c(c1)Cc1cccnc1N1CCN(C(C)=O)CC21
Mol. weight [g/mol]: 351.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	2.321		Crippen Method
mcvol	262.370	ml/mol	McGowan Method
rinpol	2980.00		NIST Webbook
rinpol	2980.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R331078&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

Latest version available from:

<https://www.chemeo.com/cid/33-232-7/Mirtazapine-M-nor-HO-2AC.pdf>

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