

Mirtazapine-M (HO-) AC

Inchi: InChI=1S/C19H21N3O2/c1-13(23)24-16-5-6-17-15(11-16)10-14-4-3-7-20-19(14)22-9-8-2
InchiKey: NVDJCIXJFASWCZ-UHFFFAOYSA-N
Formula: C19H21N3O2
SMILES: CC(=O)Oc1ccc2c(c1)Cc1ccnc1N1CCN(C)CC21
Mol. weight [g/mol]: 323.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.404		Crippen Method
mcvol	246.710	ml/mol	McGowan Method
rinpol	2650.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R331058&Units=SI>
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>

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/52-361-3/Mirtazapine-M-HO-AC.pdf>

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