

Mebhydroline M (nor), acetylated

Inchi: InChI=1S/C20H20N2O/c1-15(23)21-12-11-20-18(14-21)17-9-5-6-10-19(17)22(20)13-16-7
InchiKey: YGSUGAURHSSLFW-UHFFFAOYSA-N
Formula: C20H20N2O
SMILES: CC(=O)N1CCc2c(c3ccccc3n2Cc2ccccc2)C1
Mol. weight [g/mol]: 304.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Crippen Method
logp	3.594		Crippen Method
mcvol	240.650	ml/mol	McGowan Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		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=R120655&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/30-545-3/Mebhydroline-M-nor-acetylated.pdf>

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