

Norbamipine, acetylated

Inchi: InChI=1S/C20H24N2O/c1-17(23)21-14-12-20(13-15-21)22(19-10-6-3-7-11-19)16-18-8-4
InchiKey: LBPXYTOQUPXHCB-UHFFFAOYSA-N
Formula: C20H24N2O
SMILES: CC(=O)N1CCC(N(Cc2ccccc2)c2ccccc2)CC1
Mol. weight [g/mol]: 308.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.704		Crippen Method
mcvol	255.810	ml/mol	McGowan Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536619&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/65-648-1/Norbamipine-acetylated.pdf>

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