

Bamipine, nor-hydroxy, acetylated

Inchi: InChI=1S/C22H26N2O3/c1-17(25)23-14-12-21(13-15-23)24(16-19-6-4-3-5-7-19)20-8-10
InchiKey: LIHARFGRBZETLL-UHFFFAOYSA-N
Formula: C22H26N2O3
SMILES: CC(=O)Oc1ccc(N(Cc2ccccc2)C2CCN(C(C)=O)CC2)cc1
Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	3.629		Crippen Method
mcvol	291.430	ml/mol	McGowan Method
rinpol	3020.00		NIST Webbook
rinpol	3020.00		NIST Webbook

Sources

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=R536075&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/50-797-2/Bamipine-nor-hydroxy-acetylated.pdf>

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