Bamipine, hydroxy, acetylated

Inchi: InChI=1S/C21H26N2O2/c1-17(24)25-21-10-8-19(9-11-21)23(16-18-6-4-3-5-7-18)20-12-1
InchiKey: SZTKNXVLJZWDTP-UHFFFAOYSA-N
Formula: C21H26N2O2
SMILES: CC(=O)Oc1ccc(N(Cc2ccccc2)C2CCN(C)CC2)cc1
Mol. weight [g/mol]: 338.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	3.713		Crippen Method
mcvol	275.770	ml/mol	McGowan Method
rinpol	2620.00		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=R536040&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices