acetylepibaptifoline

Inchi: InChI=1S/C17H22N2O3/c1-11(20)22-14-5-6-18-9-12-7-13(16(18)8-14)10-19-15(12)3-2-4
InchiKey: WOXXKFZZPFAEHI-MNSOJDNVSA-N
Formula: C17H22N2O3
SMILES: CC(=O)OC1CCN2CC3CC(Cn4c3cccc4=O)C2C1
Mol. weight [g/mol]: 302.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.361		Crippen Method
mcvol	227.320	ml/mol	McGowan Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R391194&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.