

Epibaptifoline

Inchi: InChI=1S/C15H20N2O2/c18-12-4-5-16-8-10-6-11(14(16)7-12)9-17-13(10)2-1-3-15(17)19
InchiKey: AOOSKCGZYCEJX-YZVRNYIASA-N
Formula: C15H20N2O2
SMILES: O=c1cccc2n1CC1CC2CN2CCC(O)CC12
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	0.791		Crippen Method
mcvol	197.570	ml/mol	McGowan Method
rinpol	2655.00		NIST Webbook
rinpol	2658.00		NIST Webbook
rinpol	2665.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2650.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R261117&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

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