Camoensidine

Inchi: InChI=1S/C15H20N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h3,5
InchiKey: FQEQMASDZFXSJI-BPCQOVAHSA-N
Formula: C15H20N2O
SMILES: O=c1cccc2n1CC1CC2CN2CCCCC12
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.820		Crippen Method
mcvol	191.700	ml/mol	McGowan Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R261157&Units=SI
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

Legend

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