Dehydroaphylline

Inchi: InChI=1S/C15H22N2O/c18-15-12-9-11(13-5-2-4-8-17(13)15)10-16-7-3-1-6-14(12)16/h6,1
InchiKey: ZNPIGJLCHSRBBI-UHFFFAOYSA-N
Formula: C15H22N2O
SMILES: O=C1C2CC(CN3CCCC=C23)C2CCCCN12
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.997		Crippen Method
mcvol	196.000	ml/mol	McGowan Method
rinpol	2190.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R322128&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