3,5,8a-trimethyl-4,4a,8a,9-tetrahydronaphtho[2,3-b

Inchi: InChI=1S/C15H18O/c1-10-5-4-6-15(3)8-14-12(7-13(10)15)11(2)9-16-14/h4-6,9,13H,7-8H
InchiKey: AUSAHAHDEVYCOC-UHFFFAOYSA-N
Formula: C15H18O
SMILES: CC1=CC=CC2(C)Cc3occ(C)c3CC12
Mol. weight [g/mol]: 214.30
CAS: 115526-32-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.81		Crippen Method
logp	3.825		Crippen Method
mcvol	178.300	ml/mol	McGowan Method
rinpol	1645.70		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1645.70		NIST Webbook
ripol	2162.00		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=C115526324&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

ripol: Polar retention indices