3,5,8a-Trimethyl-4,6,8a,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/h4,6,9H,5,7-8H2
InchiKey: NXFJHCXGPPVGQH-UHFFFAOYSA-N
Formula: C15H18O
SMILES: CC1=C2Cc3c(C)coc3CC2(C)C=CC1
Mol. weight [g/mol]: 214.30
CAS: 631868-96-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.05		Crippen Method
logp	3.969		Crippen Method
mcvol	178.300	ml/mol	McGowan Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
ripol	2080.00		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=C631868967&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