4-Quinolinol, 4-ethynyldecahydro-1,2-dimethyl-, (2«alpha»,4«alpha»,4a«alpha»,8a«beta»)-

Other names: 4-Quinolinol, 4-ethynyldecahydro-1,2-dimethyl-, (2«alpha»,4«alpha»,4a«alpha»,8a«beta»)-

Inchi: InChI=1S/C13H21NO/c1-4-13(15)9-10(2)14(3)12-8-6-5-7-11(12)13/h1,10-12,15H,5-9H2,

InchiKey: OMBITJGEGMMNIO-VOAKCMCISA-N

Formula: C13H21NO

SMILES: C#CC1(O)CC(C)N(C)C2CCCCC21

Mol. weight [g/mol]: 207.31

CAS: 16067-80-4

Physical Properties

Property code	Value	Unit	Source
ie	7.40 ± 0.02	eV	NIST Webbook
log10ws	-2.78		Crippen Method
logp	1.634		Crippen Method
mcvol	179.560	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16067804&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/43-815-9/4-Quinolinol-4-ethynyldecahydro-1-2-dimethyl-2-alpha-4-alpha-4a-alpha-8a-b