4-Quinolinol,1-ethyl-4-ethynyldecahydro-2-methyl

Inchi: InChI=1S/C14H23NO/c1-4-14(16)10-11(3)15(5-2)13-9-7-6-8-12(13)14/h1,11-13,16H,5-10
InchiKey: ONKFFRQKKYWROK-RFGFWPKPSA-N
Formula: C14H23NO
SMILES: C#CC1(O)CC(C)N(CC)C2CCCCC21
Mol. weight [g/mol]: 221.34
CAS: 38463-54-6

Physical Properties

Property code	Value	Unit	Source
ie	7.33 ± 0.02	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	2.024		Crippen Method
mcvol	193.650	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38463546&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

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.