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-ZOBORPQBSA-N

Formula: C14H23NO

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

Mol. weight [g/mol]: 221.34

CAS: 38463-55-7

Physical Properties

Property code	Value	Unit	Source
ie	7.28 ± 0.02	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	2.024		Crippen Method
mcvol	193.650	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38463557&Units=SI

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.