

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,5-1
InchiKey:	ONKFFRQKKYWROK-SYQHCUMBSA-N
Formula:	C14H23NO
SMILES:	C#CC1(O)CC(C)N(CC)C2CCCCC21
Mol. weight [g/mol]:	221.34
CAS:	38463-56-8

Physical Properties

Property code	Value	Unit	Source
ie	7.16 ± 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/ci9903071
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=C38463568&Units=SI

Legend

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

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