

4-Quinolinol,4-ethenyl-1-ethyldecahydro-2-methyl

Inchi:	InChI=1S/C14H25NO/c1-4-14(16)10-11(3)15(5-2)13-9-7-6-8-12(13)14/h4,11-13,16H,1,5-
InchiKey:	LKEYOSUGLGHCCU-RFGFWPKPSA-N
Formula:	C14H25NO
SMILES:	C=CC1(O)CC(C)N(CC)C2CCCCC21
Mol. weight [g/mol]:	223.35
CAS:	38463-57-9

Physical Properties

Property code	Value	Unit	Source
ie	7.32 ± 0.02	eV	NIST Webbook
log10ws	-3.25		Crippen Method
logp	2.576		Crippen Method
mcvol	197.950	ml/mol	McGowan Method

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=C38463579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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