

4-Quinolinol,1,4-diethyldecahydro-2-methyl-(2«alp

Inchi:	InChI=1S/C14H27NO/c1-4-14(16)10-11(3)15(5-2)13-9-7-6-8-12(13)14/h11-13,16H,4-10H
InchiKey:	MFCNLJAJNKZFCG-ZOBORPQBSA-N
Formula:	C14H27NO
SMILES:	CCN1C(C)CC(O)(CC)C2CCCCC21
Mol. weight [g/mol]:	225.37
CAS:	38463-61-5

Physical Properties

Property code	Value	Unit	Source
ie	7.23 ± 0.02	eV	NIST Webbook
log10ws	-3.40		Crippen Method
logp	2.800		Crippen Method
mcvol	202.250	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=C38463615&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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<https://www.chemeo.com/cid/43-820-3/4-Quinolinol-1-4-diethyldecahydro-2-methyl-2-alpha-4-beta-4a-alpha-8a-beta>.

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