

4-Quinolinol, 4-ethyldecahydro-1,2-dimethyl-, (2«alpha»,4«beta»,4a«alpha»,8a«beta»)-

Other names:	4-Quinolinol, 4«alpha»-ethyl-1,2,3,4,4a«alpha»,5,6,7,8,8a«beta»-decahydro-1,2«alpha»-dimethyl-4-quinolinol, 4«beta»-ethyl-1,2,3,4,4a«beta»,5,6,7,8,8a«alpha»-decahydro-1,2«beta»-dimethyl-4-ethyl-1,2-dimethyldecahydro-4-quinolinol-, (2«alpha»,4«beta»,4a«alpha»,8a«beta»)-
Inchi:	InChI=1S/C13H25NO/c1-4-13(15)9-10(2)14(3)12-8-6-5-7-11(12)13/h10-12,15H,4-9H2,1-
InchiKey:	UKBFFPGRVCZRQZ-LOWDOPEQSA-N
Formula:	C13H25NO
SMILES:	CCC1(O)CC(C)N(C)C2CCCCC21
Mol. weight [g/mol]:	211.34
CAS:	20422-72-4

Physical Properties

Property code	Value	Unit	Source
ie	7.32 ± 0.02	eV	NIST Webbook
log10ws	-2.98		Crippen Method
logp	2.410		Crippen Method
mcvol	188.160	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=C20422724&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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