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

Other names: 4-Quinolinol, 4«alpha»-ethyl-1,2,3,4,4a«alpha»,5,6,7,8,8a«beta»-decahydro-1,2«beta»-dimethyl-
4-Quinolinol, 4«beta»-ethyl-1,2,3,4,4a«beta»,5,6,7,8,8a«alpha»-decahydro-1,2«alpha»-dimethyl-
4-Quinolinol, 4-ethyldecahydro-1,2-dimethyl-, stereoisomer
4-Ethyl-1,2-dimethyldecahydro-4-quinolinol-, (2«alpha»,4«alpha»,4a«beta»,8a«alpha»)-
4-Quinolinol, 4-ethyldecahydro-1,2-dimethyl-, (2R,4S,4aR,8aR)-rel-

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-ZDEQEGDKSA-N

Formula: C13H25NO

SMILES: CCC1(O)CC(C)N(C)C2CCCCC21

Mol. weight [g/mol]: 211.34

CAS: 20422-68-8

Physical Properties

Property code	Value	Unit	Source
ie	7.19 ± 0.02	eV	NIST Webbook
log10ws	-2.98		Crippen Method
logp	2.410		Crippen Method
mcvol	188.160	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20422688&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/57-606-6/4-Quinolinol-4-ethyldecahydro-1-2-dimethyl-2-alpha-4-alpha-4a-beta-8a-alpha
Generated by Cheméo on 2024-04-25 18:10:55.039976892 +0000 UTC m=+16357903.960554207.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.