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

Other names: 4-Quinolinol, 1,2,3,4,4a«alpha»,5,6,7,8,8a«beta»-decahydro-1,2«beta»-dimethyl-4«beta»-vinyl-
4-Quinolinol, decahydro-1,2-dimethyl-4-vinyl-, stereoisomer
4-Quinolinol, 1,2,3,4,4a«alpha»,5,6,7,8,8a«beta»-decahydro-1,2«beta»-dimethyl-4«alpha»-vinyl-
4-Quinolinol, 4-ethenyldecahydro-1,2-dimethyl-, (2R,4R,4aR,8aR)-rel-

Inchi: InChI=1S/C13H23NO/c1-4-13(15)9-10(2)14(3)12-8-6-5-7-11(12)13/h4,10-12,15H,1,5-9H

InchiKey: DNTLHLDYMDJBDF-LPWJVIDDSA-N

Formula: C13H23NO

SMILES: C=CC1(O)CC(C)N(C)C2CCCCC21

Mol. weight [g/mol]: 209.33

CAS: 20431-91-8

Physical Properties

Property code	Value	Unit	Source
ie	7.26 ± 0.02	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.186		Crippen Method
mcvol	183.860	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=C20431918&Units=SI

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

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume