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

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|---|---|
| **Other names:** | 4-Quinolinol, 1,2,3,4,4a,5,6,7,8,8a-decahydro-1,2-dimethyl-4«beta»-vinyl-4-Quinolinol, decahydro-1,2-dimethyl-4-vinyl-, stereoisomer<br>4-Quinolinol, 1,2,3,4,4a«alpha»,5,6,7,8,8a«beta»-decahydro-1,2«alpha»-dimethyl-4«alpha»-vinyl-4-Quinolinol, 4-ethenyldecahydro-1,2-dimethyl-, (2R,4S,4aS,8aS)-rel-<br>1,2-Dimethyl-4-vinyldecahydro-4-quinolinol, (2R,4S,4aS,8aS)-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-MROQNXINSA-N |
| **Formula:** | C13H23NO |
| **SMILES:** | C=CC1(O)CC(C)N(C)C2CCCCC21 |
| **Mol. weight [g/mol]:** | 209.33 |
| **CAS:** | 20431-95-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 7.39 ± 0.02 | eV | NIST Webbook |
| log10ws | -2.83 | | Crippen Method |
| logp | 2.186 | | Crippen Method |
| mcvol | 183.860 | ml/mol | McGowan Method |

## Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C20431952&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