

Alpha-quinolyl-ethanol

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|-----------------------------|--|
| Other names: | quinoline-2-ethanol |
| Inchi: | InChI=1S/C11H11NO/c13-8-7-10-6-5-9-3-1-2-4-11(9)12-10/h1-6,13H,7-8H2 |
| InchiKey: | VPDAGUVEZGEHJJ-UHFFFAOYSA-N |
| Formula: | C11H11NO |
| SMILES: | OCCc1ccc2ccccc2n1 |
| Mol. weight [g/mol]: | 173.21 |
| CAS: | 1011-50-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.11 | | Crippen Method |
| logp | 1.770 | | Crippen Method |
| mcvol | 138.480 | 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=C1011503&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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