

2-Pyrrolidineethanol

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|-----------------------------|--|
| Other names: | pyrrolidine-2-ethanol |
| Inchi: | InChI=1S/C6H9NO/c8-5-3-6-2-1-4-7-6/h1-2,4,7-8H,3,5H2 |
| InchiKey: | XBVPIPOORLGFGK-UHFFFAOYSA-N |
| Formula: | C6H9NO |
| SMILES: | OCCc1ccc[nH]1 |
| Mol. weight [g/mol]: | 111.14 |
| CAS: | 19432-88-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -0.76 | | Crippen Method |
| logp | 0.068 | | Crippen Method |
| mcvol | 91.790 | ml/mol | McGowan Method |
| rinpol | 986.00 | | NIST Webbook |
| rinpol | 997.00 | | NIST Webbook |
| rinpol | 986.00 | | NIST Webbook |

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=C19432883&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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

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