# 1H-Pyrrole, 2-ethyl-1-methyl

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|---|---|
| **Inchi:** | InChI=1S/C7H11N/c1-3-7-5-4-6-8(7)2/h4-6H,3H2,1-2H3 |
| **InchiKey:** | NRFLRWJZUPDSLT-UHFFFAOYSA-N |
| **Formula:** | C7H11N |
| **SMILES:** | CCc1cccn1C |
| **Mol. weight [g/mol]:** | 109.17 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.56 | | Crippen Method |
| logp | 1.587 | | Crippen Method |
| mcvol | 100.010 | ml/mol | McGowan Method |
| rinpol | 967.00 | | NIST Webbook |
| rinpol | 967.00 | | NIST Webbook |

## Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=R62980&Units=SI |

## 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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