

1H-Pyrrole, 4-ethyl-2,3-dimethyl-

| | |
|-----------------------------|--|
| Other names: | 2,3-Dimethyl-4-ethylpyrrole |
| Inchi: | InChI=1S/C8H13N/c1-4-8-5-9-7(3)6(8)2/h5,9H,4H2,1-3H3 |
| InchiKey: | WGUZBCNNSVWXTR-UHFFFAOYSA-N |
| Formula: | C8H13N |
| SMILES: | CCc1c[nH]c(C)c1C |
| Mol. weight [g/mol]: | 123.20 |
| CAS: | 491-18-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.44 | | Crippen Method |
| logp | 1.712 | | Crippen Method |
| mcvol | 114.100 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 386.20 | K | 2.10 | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=C491189&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcpvol: | McGowan's characteristic volume |
| tbrp: | Boiling point at reduced pressure |

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