

1H-Pyrrole-2-carboxaldehyde, 1-ethyl-

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| Other names: | 1-Ethyl-1H-pyrrole-2-carboxaldehyde 1-Ethyl-1H-pyrrole-2-carboxyaldehyde 1-Ethyl-2-formyl-1H-pyrrole 1-Ethyl-2-formylpyrrole 1-Ethyl-2-pyrrolecarbaldehyde |
| Inchi: | InChI=1S/C7H9NO/c1-2-8-5-3-4-7(8)6-9/h3-6H,2H2,1H3 |
| InchiKey: | DVLGEHCERRWDIX-UHFFFAOYSA-N |
| Formula: | C7H9NO |
| SMILES: | CCn1cccc1C=O |
| Mol. weight [g/mol]: | 123.15 |
| CAS: | 2167-14-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.97 | | Crippen Method |
| logp | 1.321 | | Crippen Method |
| mcvol | 101.580 | ml/mol | McGowan Method |
| rinpol | 1046.00 | | NIST Webbook |
| rinpol | 1067.00 | | NIST Webbook |
| rinpol | 1039.00 | | NIST Webbook |
| rinpol | 1067.00 | | NIST Webbook |
| ripol | 1610.00 | | NIST Webbook |
| ripol | 1610.00 | | NIST Webbook |
| ripol | 1610.00 | | NIST Webbook |
| ripol | 1566.00 | | NIST Webbook |
| ripol | 1562.00 | | NIST Webbook |
| ripol | 1616.00 | | NIST Webbook |
| ripol | 1616.00 | | NIST Webbook |
| ripol | 1610.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2167148&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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