

N-(2-Hydroxyethyl)-2-pyrrolidone

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|-----------------------------|--|
| Other names: | 1-(2-Hydroxyethyl)-2-pyrrolidone 2-Pyrrolidinone, 1-(2-hydroxyethyl)- N-2-Hydroxyethylpyrrolidin-2-one 1-(2-Hydroxyethyl)-2-pyrrolidinone 1-(2-hydroxyethyl)pyrrolidin-2-one |
| Inchi: | InChI=1S/C6H11NO2/c8-5-4-7-3-1-2-6(7)9/h8H,1-5H2 |
| InchiKey: | WDQFELCEOPFLCZ-UHFFFAOYSA-N |
| Formula: | C6H11NO2 |
| SMILES: | O=C1CCCN1CCO |
| Mol. weight [g/mol]: | 129.16 |
| CAS: | 3445-11-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | 0.16 | | Crippen Method |
| logp | -0.399 | | Crippen Method |
| mcvol | 101.960 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 414.20 | K | 0.40 | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3445112&Units=SI |
| 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 |

Legend

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

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