

2-Pyrrolidinone, 1-phenyl-

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|-----------------------------|---|
| Other names: | N-Phenyl-2-pyrrolidinone N-Phenyl-2-pyrrolidone 1-Phenyl-2-pyrrolidinone N-Phenyl pyrrolidone 1-Phenyl-2-pyrrolidone 1-Phenyl-pyrrolidin-2-one |
| Inchi: | InChI=1S/C10H11NO/c12-10-7-4-8-11(10)9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2 |
| InchiKey: | JMVIVASFFKKFKQK-UHFFFAOYSA-N |
| Formula: | C10H11NO |
| SMILES: | O=C1CCCN1c1ccccc1 |
| Mol. weight [g/mol]: | 161.20 |
| CAS: | 4641-57-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.89 | | Crippen Method |
| logp | 1.813 | | Crippen Method |
| mcpvol | 128.690 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 396.20 | K | 0.03 | 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=C4641570&Units=SI |

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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