

# 1,2-bis-(1-Pyrrolidiny1)-1-buten-3-one

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C12H20N2O/c1-10(15)12(14-7-2-3-8-14)9-11-5-4-6-13-11/h9,11,13H,2-8H2,1H |
| <b>InchiKey:</b>            | KIELAOHVFOBDLD-XFXZXTDPSA-N  |
| <b>Formula:</b>             | C12H20N2O  |
| <b>SMILES:</b>              | CC(=O)C(=CC1CCCN1)N1CCCC1  |
| <b>Mol. weight [g/mol]:</b> | 208.30   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.14   |        | Crippen Method |
| logp          | 1.307   |        | Crippen Method |
| mcvol         | 175.450 | ml/mol | McGowan Method |
| ripol         | 2726.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R532459&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R532459&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

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

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