

# 1,2,3,4,6,7,8,9,10,11-Decahydro-5,11a-diaza-cycloocta-b-naphthalen-12-one

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C14H20N2O/c17-14-11-7-4-5-8-12(11)15-13-9-3-1-2-6-10-16(13)14/h1-10H2 |
| <b>InchiKey:</b>            | WCFODMJXNQITOI-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C14H20N2O  |
| <b>SMILES:</b>              | O=c1c2c(nc3n1CCCCC3)CCCC2  |
| <b>Mol. weight [g/mol]:</b> | 232.32   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.96   |        | Crippen Method |
| logp          | 2.239   |        | Crippen Method |
| mcvol         | 188.470 | ml/mol | McGowan Method |
| rinpol        | 2165.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <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=R318248&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R318248&amp;Units=SI</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>rinpol:</b>  | Non-polar retention indices         |

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