

# 10-Methoxy-14-methyl-5-oxo-5,7,8,14-tetrahydro-i

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C20H17N3O2/c1-22-17-6-4-3-5-14(17)20(24)23-10-9-13-15-11-12(25-2)7-8-16 |
| <b>InchiKey:</b>            | UBJRXOPIHBJHV-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C20H17N3O2   |
| <b>SMILES:</b>              | COc1ccc2c(c1)=C1CCN3C(=O)c4ccccc4N(C)C3=C1N=2                                    |
| <b>Mol. weight [g/mol]:</b> | 331.37   |
| <b>CAS:</b>                 | 477-40-7   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.41   |        | Crippen Method |
| logp          | 1.644   |        | Crippen Method |
| mcvol         | 241.340 | ml/mol | McGowan Method |

## 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=C477407&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C477407&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     |

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