

# 3-Methyl-1-benzoyl-(1H)-1,2-diazepine

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C13H12N2O/c1-11-7-5-6-10-15(14-11)13(16)12-8-3-2-4-9-12/h2-10H,1H3 |
| <b>InchiKey:</b>            | PHQSCYFZZWMASY-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C13H12N2O   |
| <b>SMILES:</b>              | CC1=NN(C(=O)c2ccccc2)C=CC=C1  |
| <b>Mol. weight [g/mol]:</b> | 212.25  |
| <b>CAS:</b>                 | 69298-66-4  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.54   |        | Crippen Method |
| logp          | 2.588   |        | Crippen Method |
| mcvol         | 168.040 | 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=C69298664&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C69298664&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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