

# Benzoxazole, 2-phenyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2-phenylbenzo[d]oxazole<br>2-phenylbenzoxazole                      |
| <b>Inchi:</b>               | InChI=1S/C13H9NO/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9H |
| <b>InchiKey:</b>            | FIISKTXZUZBTRC-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C13H9NO   |
| <b>SMILES:</b>              | <chem>c1ccc(-c2nc3ccccc3o2)cc1</chem>                               |
| <b>Mol. weight [g/mol]:</b> | 195.22  |
| <b>CAS:</b>                 | 833-50-1  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -9.38   |        | Crippen Method |
| logp          | 3.495   |        | Crippen Method |
| mvol          | 147.200 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit   | Temperature [K] | Source  |
|---------------|-------|--------|-----------------|---|
| hvapt         | 90.90 | kJ/mol | 298.15          | Thermochemical and conformational study of optical active phenylbenzazole derivatives |

## Sources

|   |   |
|---|---|
| <b>Crippen Method:</b>  | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Thermochemical and conformational study of optical active phenylbenzazole derivatives:</b> | <a href="https://www.doi.org/10.1016/j.jct.2017.08.017">https://www.doi.org/10.1016/j.jct.2017.08.017</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=C833501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C833501&amp;Units=SI</a> |
| <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>                                 |

# Legend

|                 |   |
|-----------------|---|
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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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