

# 1H-Indole, 2,3-dihydro-1,2-dimethyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Indoline, 1,2-dimethyl-<br>1,2-Dimethylindoline<br>1,2-Dimethyl-2,3-dihydro-1H-indole |
| <b>Inchi:</b>               | InChI=1S/C10H13N/c1-8-7-9-5-3-4-6-10(9)11(8)2/h3-6,8H,7H2,1-2H3                       |
| <b>InchiKey:</b>            | ZDOWGOCJXFRDOM-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C10H13N   |
| <b>SMILES:</b>              | CC1Cc2ccccc2N1C   |
| <b>Mol. weight [g/mol]:</b> | 147.22  |
| <b>CAS:</b>                 | 26216-93-3  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.19   |        | Crippen Method |
| logp          | 2.067   |        | Crippen Method |
| mcvol         | 127.120 | ml/mol | McGowan Method |

## 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=C26216933&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26216933&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>                                     |
| <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     |

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