

5,6-Dehydromultiflorine

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|----------------------|---|
| Inchi: | InChI=1S/C15H20N2O/c18-13-4-6-17-9-11-7-12(15(17)8-13)10-16-5-2-1-3-14(11)16/h4,6 |
| InchiKey: | SJRGHHOFXSLZOB-ORHYLEIMSA-N |
| Formula: | C15H20N2O |
| SMILES: | O=c1ccn2c(c1)C1CC(C2)C2CCCCN2C1 |
| Mol. weight [g/mol]: | 244.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.56 | | Crippen Method |
| logp | 1.820 | | Crippen Method |
| mcvol | 191.700 | ml/mol | McGowan Method |
| rinpol | 2110.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R557072&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpol: | Non-polar retention indices |

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<https://www.chemeo.com/cid/41-612-6/5-6-Dehydromultiflorine.pdf>

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