

bis-(4-Methoxyphenyl)-(3-pyridyl)carbinol

Inchi: InChI=1S/C20H19NO3/c1-23-18-9-5-15(6-10-18)20(22,17-4-3-13-21-14-17)16-7-11-19(2)
InchiKey: QKASDQKKOSHQML-UHFFFAOYSA-N
Formula: C20H19NO3
SMILES: COc1ccc(C(O)(c2ccc(OC)cc2)c2cccnc2)cc1
Mol. weight [g/mol]: 321.37

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.73 | | Crippen Method |
| logp | 3.383 | | Crippen Method |
| mcvol | 248.970 | ml/mol | McGowan Method |
| rinpol | 2669.00 | | NIST Webbook |
| ripol | 3800.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537721&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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