

Phenyl-(4-chlorophenyl)-(2-pyridyl)carbinol

Inchi: InChI=1S/C18H14ClNO/c19-16-11-9-15(10-12-16)18(21,14-6-2-1-3-7-14)17-8-4-5-13-20
InchiKey: COFNBGMKTMAFRO-UHFFFAOYSA-N
Formula: C18H14ClNO
SMILES: OC(c1ccccc1)(c1ccc(Cl)cc1)c1cccn1
Mol. weight [g/mol]: 295.76

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.17 | | Crippen Method |
| logp | 4.019 | | Crippen Method |
| mcvol | 221.290 | ml/mol | McGowan Method |
| rinpol | 2349.00 | | NIST Webbook |
| ripol | 3357.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R537810&Units=SI>

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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