Phenyl-(4-chlorophenyl)-(3-pyridyl)carbinol

Inchi: InChI=1S/C18H14ClNO/c19-17-10-8-15(9-11-17)18(21,14-5-2-1-3-6-14)16-7-4-12-20-13-
InchiKey: GMUXFNGMJVMSHJ-UHFFFAOYSA-N
Formula: C18H14ClNO
SMILES: OC(c1ccccc1)(c1ccc(Cl)cc1)c1cccnc1
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	2610.00		NIST Webbook
ripol	4102.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R537825&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