Diphenyl-(3-pyridyl)carbinol

Inchi: InChI=1S/C18H15NO/c20-18(15-8-3-1-4-9-15,16-10-5-2-6-11-16)17-12-7-13-19-14-17/h1
InchiKey: GAGJIFCXHADNEC-UHFFFAOYSA-N
Formula: C18H15NO
SMILES: OC(c1ccccc1)(c1ccccc1)c1cccnc1
Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	3.366		Crippen Method
mcvol	209.050	ml/mol	McGowan Method
rinpol	2254.00		NIST Webbook
rinpol	2254.00		NIST Webbook
ripol	3507.00		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=R537761&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