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

Inchi: InChI=1S/C18H15NO2/c20-17-10-8-15(9-11-17)18(21,14-5-2-1-3-6-14)16-7-4-12-19-13-
InchiKey: YEXGCRWNATVUMN-UHFFFAOYSA-N
Formula: C18H15NO2
SMILES: Oc1ccc(C(O)(c2ccccc2)c2cccnc2)cc1
Mol. weight [g/mol]: 277.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	3.071		Crippen Method
mcvol	214.920	ml/mol	McGowan Method
rinpol	2556.00		NIST Webbook
ripol	3959.00		NIST Webbook
ripol	3959.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537845&Units=SI
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

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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