

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

Inchi: InChI=1S/C19H17NO2/c1-22-18-11-9-16(10-12-18)19(21,15-6-3-2-4-7-15)17-8-5-13-20-
InchiKey: SDFCLRPPKKXECJ-UHFFFAOYSA-N
Formula: C19H17NO2
SMILES: COc1ccc(C(O)(c2ccccc2)c2ccnc2)cc1
Mol. weight [g/mol]: 291.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	3.374		Crippen Method
mcvol	229.010	ml/mol	McGowan Method
rinpol	2516.00		NIST Webbook
ripol	3832.00		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=R537850&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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