Phenyl-(2-chlorophenyl)-(1-imidazolyl) carbinol

Other names: Phenyl-(2-chlorophenyl)-imidazolyl carbinol
Inchi: InChI=1S/C16H13ClN2O/c17-15-9-5-4-8-14(15)16(20,19-11-10-18-12-19)13-6-2-1-3-7-1
InchiKey: NRUPNNHIPZMULJ-UHFFFAOYSA-N
Formula: C16H13ClN2O
SMILES: OC(c1ccccc1)(c1ccccc1Cl)n1ccnc1
Mol. weight [g/mol]: 284.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	3.278		Crippen Method
mcvol	207.390	ml/mol	McGowan Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
ripol	3236.00		NIST Webbook
ripol	3236.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537885&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