Phenyl-(4-chlorophenyl)-(5-pyrimidinyl)carbinol

Inchi: InChI=1S/C17H13ClN2O/c18-16-8-6-14(7-9-16)17(21,13-4-2-1-3-5-13)15-10-19-12-20-1
InchiKey: QJYBUDJACCWKFB-UHFFFAOYSA-N
Formula: C17H13ClN2O
SMILES: OC(c1ccccc1)(c1ccc(Cl)cc1)c1cncnc1
Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	3.414		Crippen Method
mcvol	217.180	ml/mol	McGowan Method
ripol	3822.00		NIST Webbook
ripol	3822.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537909&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.