

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

Inchi: InChI=1S/C17H13FN2O/c18-16-8-6-14(7-9-16)17(21,13-4-2-1-3-5-13)15-10-19-12-20-11
InchiKey: SJIBRANLJCPUBV-UHFFFAOYSA-N
Formula: C17H13FN2O
SMILES: OC(c1ccccc1)(c1ccc(F)cc1)c1cncnc1
Mol. weight [g/mol]: 280.30

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.58 | | Crippen Method |
| logp | 2.900 | | Crippen Method |
| mcvol | 206.710 | ml/mol | McGowan Method |
| ripol | 3574.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R537914&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/74-470-8/Phenyl-4-fluorophenyl-5-pyrimidinyl-carbinol.pdf>

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