

(2-Fluorophenyl)-(4-chlorophenyl)-(5-pyrimidinyl)

Inchi: InChI=1S/C17H12ClFN2O/c18-14-7-5-12(6-8-14)17(22,13-9-20-11-21-10-13)15-3-1-2-4-
InchiKey: HRFUFIMTPKTRSV-UHFFFAOYSA-N
Formula: C17H12ClFN2O
SMILES: OC(c1ccc(Cl)cc1)(c1cncnc1)c1ccccc1F
Mol. weight [g/mol]: 314.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Crippen Method
logp	3.553		Crippen Method
mcvol	218.950	ml/mol	McGowan Method
rinpol	2358.00		NIST Webbook
rinpol	2358.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537870&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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