1-[(4-chlorophenyl)methyl]-5-fluoropyrimidine-2,4

Inchi: InChI=1S/C11H8ClFN2O2/c12-8-3-1-7(2-4-8)5-15-6-9(13)10(16)14-11(15)17/h1-4,6H,5H

InchiKey: FWLNZTGNVCRKCU-UHFFFAOYSA-N

Formula: C11H8ClFN2O2

SMILES: O=c1[nH]c(=O)n(Cc2ccc(Cl)cc2)cc1F

Mol. weight [g/mol]: 254.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Aqueous Solubility Prediction Method
logp	0.895		Crippen Method
mcvol	164.040	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume