5-fluoro-1-[(4-methylphenyl)methyl]pyrimidine-2,4

Inchi: InChI=1S/C12H11FN2O2/c1-8-2-4-9(5-3-8)6-15-7-10(13)11(16)14-12(15)17/h2-5,7H,6H2

InchiKey: POACFNLCTNKXFD-UHFFFAOYSA-N

Formula: C12H11FN2O2

SMILES: Cc1ccc(Cn2cc(F)c(=O)[nH]c2=O)cc1

Mol. weight [g/mol]: 234.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Aqueous Solubility Prediction Method
logp	0.551		Crippen Method
mcvol	165.890	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