

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/ci9903071
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

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