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

Inchi: InChI=1S/C12H11FN2O3/c1-18-9-4-2-8(3-5-9)6-15-7-10(13)11(16)14-12(15)17/h2-5,7H,
InchiKey: IWTFDHOAOPEINT-UHFFFAOYSA-N
Formula: C12H11FN2O3
SMILES: COc1ccc(Cn2cc(F)c(=O)[nH]c2=O)cc1
Mol. weight [g/mol]: 250.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Aqueous Solubility Prediction Method
logp	0.251		Crippen Method
mcvol	171.760	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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