

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:	IWTFDHOAPEINT-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/AqueousDataset002.xlsx>

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

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