

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

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/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

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

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