5-fluoro-1-(phenylmethyl)pyrimidine-2,4-dione

Inchi: InChI=1S/C11H9FN2O2/c12-9-7-14(11(16)13-10(9)15)6-8-4-2-1-3-5-8/h1-5,7H,6H2,(H,1
InchiKey: DOLBESUBPIZBQY-UHFFFAOYSA-N
Formula: C11H9FN2O2
SMILES: O=c1[nH]c(=O)n(Cc2ccccc2)cc1F
Mol. weight [g/mol]: 220.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Aqueous Solubility Prediction Method
logp	0.242		Crippen Method
mcvol	151.800	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