

5-fluoro-1-(oxolan-2-yl)pyrimidine-2,4-dione

Inchi:	InChI=1S/C8H9FN2O3/c9-5-4-11(6-2-1-3-14-6)8(13)10-7(5)12/h4,6H,1-3H2,(H,10,12,13)
InchiKey:	WFWLQNSHRPWKFK-UHFFFAOYSA-N
Formula:	C8H9FN2O3
SMILES:	O=c1[nH]c(=O)n(C2CCCO2)cc1F
Mol. weight [g/mol]:	200.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Aqueous Solubility Prediction Method
logp	-0.497		Crippen Method
mcvol	128.300	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/ci9903071>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/100-283-6/5-fluoro-1-oxolan-2-yl-pyrimidine-2-4-dione.pdf>

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