4-amino-1-[5-(hydroxymethyl)oxolan-2-yl]pyrimidi

Inchi: InChI=1S/C9H13N3O3/c10-7-3-4-12(9(14)11-7)8-2-1-6(5-13)15-8/h3-4,6,8,13H,1-2,5H2,
InchiKey: WREGKURFCTUGRC-UHFFFAOYSA-N
Formula: C9H13N3O3
SMILES: Nc1ccn(C2CCC(CO)O2)c(=O)n1
Mol. weight [g/mol]: 211.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.43		Aqueous Solubility Prediction Method
logp	-0.505		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
tf	490.65	K	Aqueous Solubility Prediction Method

Sources

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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