7H-pyrrolo[2,3-d]pyrimidine, 4-amino-7-[3-(hydroxymethyl)cyclopentyl]-

Inchi: InChI=1S/C12H16N4O/c13-11-10-3-4-16(12(10)15-7-14-11)9-2-1-8(5-9)6-17/h3-4,7-9,17

InchiKey: XVEJYMVNCBBYQY-UHFFFAOYSA-N

Formula: C12H16N4O

SMILES: Nc1ncnc2c1ccn2C1CCC(CO)C1

Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	1.347		Crippen Method
mcvol	175.950	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009940&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume