

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:	XVEJYMVNCCBBYQY-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.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/54-652-8/7H-pyrrolo-2-3-d-pyrimidine-4-amino-7-3-hydroxymethyl-cyclopentyl.pdf>

Generated by Cheméo on 2024-05-03 21:10:18.989709005 +0000 UTC m=+17059867.910286341.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.