6H-Pyrido[2,1-b]quinazolin-6-one, 7,8,9,10-tetrahydro-6-methyl

Inchi: InChI=1S/C13H14N2O/c1-9-5-4-8-12-14-11-7-3-2-6-10(11)13(16)15(9)12/h4-5,8H,2-3,6-

InchiKey: VFPWMBLVVYEHQO-UHFFFAOYSA-N

Formula: C13H14N2O

SMILES: Cc1cccc2nc3c(c(=O)n12)CCCC3

Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	1.882		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R119883&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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