11H-Pyrido[2,1-b]quinazolin-11-one, 1,2,3,4,6,7,8,9-octahydro, 9-methyl

Inchi: InChI=1S/C13H18N2O/c1-9-5-4-6-10-12(9)13(16)15-8-3-2-7-11(15)14-10/h9H,2-8H2,1H

InchiKey: MIWWVVZYYMXOCI-UHFFFAOYSA-N

Formula: C13H18N2O

SMILES: CC1CCCc2nc3n(c(=O)c21)CCCC3

Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	2.019		Crippen Method
mcvol	174.380	ml/mol	McGowan Method
rinpol	2071.00		NIST Webbook
rinpol	2071.00		NIST Webbook

Sources

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=R64130&Units=SI

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

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.