9-Methyl-6,7,8,9-tetrahydro-pyrido[2,1-b]quinazolin-11-one

Inchi: InChI=1S/C13H14N2O/c1-9-5-4-6-10-12(9)14-11-7-2-3-8-15(11)13(10)16/h2-3,7-9H,4-6H

InchiKey: XPFJRMNRQHCORN-UHFFFAOYSA-N

Formula: C13H14N2O

SMILES: CC1CCCc2c1nc1ccccn1c2=O

Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	2.134		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook

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=R173723&Units=SI

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.