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

Inchi: InChI=1S/C13H10N2O/c1-9-6-7-12-14-11-5-3-2-4-10(11)13(16)15(12)8-9/h2-8H,1H3
InchiKey: SWAMQXRVHXAAHQ-UHFFFAOYSA-N
Formula: C13H10N2O
SMILES: Cc1ccc2nc3ccccc3c(=O)n2c1
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	2.156		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
rinpol	2058.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	2058.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R173456&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices