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

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

InchiKey: OXJMZIISYRVYTE-UHFFFAOYSA-N

Formula: C13H14N2O

SMILES: CC1CCc2c(nc3ccccn3c2=O)C1

Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	1.819		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2123.00		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=R119907&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

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