2,3-Dihydro-1H-pyrrolo[2,1-b]quinazolin-9-one

Other names: 3H-Quinazolin-4-one, 2,3-trimethyleno
Inchi: InChI=1S/C11H10N2O/c14-11-8-4-1-2-5-9(8)12-10-6-3-7-13(10)11/h1-2,4-5H,3,6-7H2
InchiKey: VARHXCYGZKSOOO-UHFFFAOYSA-N
Formula: C11H10N2O
SMILES: O=c1c2ccccc2nc2n1CCC2
Mol. weight [g/mol]: 186.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	1.343		Crippen Method
mcvol	137.600	ml/mol	McGowan Method
rinpol	1958.00		NIST Webbook
rinpol	1973.00		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1958.00		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=R119823&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