3H-Pyrimidin-4-one, 2,3-pentamethyleno-5,6-tetramethyleno

Other names: 1,3,4,6,7,8,9,10-Octahydro-2H-azepino[2,1-b]quinazolin-12-one
Inchi: InChI=1S/C13H18N2O/c16-13-10-6-3-4-7-11(10)14-12-8-2-1-5-9-15(12)13/h1-9H2
InchiKey: QFNBTCDQRILBND-UHFFFAOYSA-N
Formula: C13H18N2O
SMILES: O=c1c2c(nc3n1CCCCC3)CCCC2
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	1.849		Crippen Method
mcvol	174.380	ml/mol	McGowan Method
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R119769&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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