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

Other names: 2,3,5,6,7,8-Hexahydro-1H-4,8a-diaza-cyclopenta[b]naphthalen-9-one
Inchi: InChI=1S/C11H14N2O/c14-11-8-4-3-5-9(8)12-10-6-1-2-7-13(10)11/h1-7H2
InchiKey: GMFURYYNPXBKGY-UHFFFAOYSA-N
Formula: C11H14N2O
SMILES: O=c1c2c(nc3n1CCCC3)CCC2
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.068		Crippen Method
mcvol	146.200	ml/mol	McGowan Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1961.00		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=R119789&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

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