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

Inchi: InChI=1S/C12H16N2O/c1-8-4-2-5-9-11(8)12(15)14-7-3-6-10(14)13-9/h8H,2-7H2,1H3
InchiKey: XFIHQKQYUXTDFI-UHFFFAOYSA-N
Formula: C12H16N2O
SMILES: CC1CCCc2nc3n(c(=O)c21)CCC3
Mol. weight [g/mol]: 204.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	1.629		Crippen Method
mcvol	160.290	ml/mol	McGowan Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R119794&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.