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

Other names: 1,2,3,5,6,7,8,9-Octahydro-4,9a-diaza-cyclohepta[f]inden-10-one
Inchi: InChI=1S/C12H16N2O/c15-12-9-5-4-6-10(9)13-11-7-2-1-3-8-14(11)12/h1-8H2
InchiKey: SPMNQNOXHNXYSJ-UHFFFAOYSA-N
Formula: C12H16N2O
SMILES: O=c1c2c(nc3n1CCCCC3)CCC2
Mol. weight [g/mol]: 204.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	1.458		Crippen Method
mcvol	160.290	ml/mol	McGowan Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
rinpol	2003.00		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=R119774&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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