

1,5-Dimethyl-5-(6-oxocyclohexen-1-yl)hexahydropyrimidin-2(1H)-one

Inchi: InChI=1S/C12H14N2O4/c1-13-10(16)9(11(17)14(2)12(13)18)7-5-3-4-6-8(7)15/h5,9H,3-4H2
InchiKey: AWYYJIQSOSIDPA-UHFFFAOYSA-N
Formula: C12H14N2O4
SMILES: CN1C(=O)C(C2=CCCCC2=O)C(=O)N(C)C1=O
Mol. weight [g/mol]: 250.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	0.332		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R577690&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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