2-Methyl-5,5-pentamethylene-4-propionyl-1,3,4-ox

Inchi: InChI=1S/C11H18N2O2/c1-3-10(14)13-11(15-9(2)12-13)7-5-4-6-8-11/h3-8H2,1-2H3
InchiKey: OQMPPZLCWSURLX-UHFFFAOYSA-N
Formula: C11H18N2O2
SMILES: CCC(=O)N1N=C(C)OC12CCCCC2
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.249		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116626&Units=SI
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

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.