5,5-Pentamethylene-2-phenyl-4-propionyl-1,3,4-ox

Inchi: InChI=1S/C16H20N2O2/c1-2-14(19)18-16(11-7-4-8-12-16)20-15(17-18)13-9-5-3-6-10-13
InchiKey: MFDMOLUXKFKYPG-UHFFFAOYSA-N
Formula: C16H20N2O2
SMILES: CCC(=O)N1N=C(c2ccccc2)OC12CCCCC2
Mol. weight [g/mol]: 272.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.277		Crippen Method
mcvol	213.920	ml/mol	McGowan Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116700&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.