5,5-Pentamethylene-4-benzoyl-1,3,4-oxadiazoline

Inchi: InChI=1S/C14H16N2O2/c17-13(12-7-3-1-4-8-12)16-14(18-11-15-16)9-5-2-6-10-14/h1,3-4
InchiKey: YMJLNLMIDKBGMR-UHFFFAOYSA-N
Formula: C14H16N2O2
SMILES: O=C(c1ccccc1)N1N=COC12CCCCC2
Mol. weight [g/mol]: 244.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.763		Crippen Method
mcvol	185.740	ml/mol	McGowan Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116720&Units=SI

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.