5,5-Pentamethylene-4-propionyl-1,3,4-oxadiazolin

Inchi: InChI=1S/C10H16N2O2/c1-2-9(13)12-10(14-8-11-12)6-4-3-5-7-10/h8H,2-7H2,1H3
InchiKey: KERVMRYZNUFBAX-UHFFFAOYSA-N
Formula: C10H16N2O2
SMILES: CCC(=O)N1N=COC12CCCCC2
Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.859		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		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=R116735&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.