5-Ethyl-5-methyl-4-acetyl-1,3,4-oxadiazoline

Inchi: InChI=1S/C7H12N2O2/c1-4-7(3)9(6(2)10)8-5-11-7/h5H,4H2,1-3H3
InchiKey: ZHCHSWANBCUERS-UHFFFAOYSA-N
Formula: C7H12N2O2
SMILES: CCC1(C)OC=NN1C(C)=O
Mol. weight [g/mol]: 156.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Crippen Method
logp	0.935		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
rinpol	1050.00		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=R116775&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