5,5-Diethyl-2-methyl-4-acetyl-1,3,4-oxadiazoline

Inchi: InChI=1S/C9H16N2O2/c1-5-9(6-2)11(8(4)12)10-7(3)13-9/h5-6H2,1-4H3
InchiKey: XFWDVGXVLDIBML-UHFFFAOYSA-N
Formula: C9H16N2O2
SMILES: CCC1(CC)OC(C)=NN1C(C)=O
Mol. weight [g/mol]: 184.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	1.715		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
rinpol	1190.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116646&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