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

Inchi: InChI=1S/C9H16N2O2/c1-5-8-10-11(7(3)12)9(4,6-2)13-8/h5-6H2,1-4H3
InchiKey: HAEDCTZNNKWZKO-UHFFFAOYSA-N
Formula: C9H16N2O2
SMILES: CCC1=NN(C(C)=O)C(C)(CC)O1
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	1200.00		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=R296292&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