

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
rinpole	1200.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpole:	Non-polar retention indices

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