

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/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=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

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