

2,5-Diethyl-5-methyl-4-propionyl-1,3,4-oxadiazolin

Inchi:	InChI=1S/C10H18N2O2/c1-5-8-11-12(9(13)6-2)10(4,7-3)14-8/h5-7H2,1-4H3
InchiKey:	JTVMBQKYGJWTCC-UHFFFAOYSA-N
Formula:	C10H18N2O2
SMILES:	CCC(=O)N1N=C(CC)OC1(C)CC
Mol. weight [g/mol]:	198.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	2.105		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
rinpola	1280.00		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=R116542&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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