

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

Inchi: InChI=1S/C10H18N2O2/c1-5-9(13)12-10(6-2,7-3)14-8(4)11-12/h5-7H2,1-4H3
InchiKey: JORVTBGCFGPJRC-UHFFFAOYSA-N
Formula: C10H18N2O2
SMILES: CCC(=O)N1N=C(C)OC1(CC)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
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R116651&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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