

2-Methyl-5,5-pentamethylene-4-acetyl-1,3,4-oxadiazole

Inchi: InChI=1S/C10H16N2O2/c1-8-11-12(9(2)13)10(14-8)6-4-3-5-7-10/h3-7H2,1-2H3
InchiKey: JZACNBZOHCFPCL-UHFFFAOYSA-N
Formula: C10H16N2O2
SMILES: CC(=O)N1N=C(C)OC12CCCCC2
Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.859		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R116611&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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