2,5,5-Trimethyl-4-acetyl-1,3,4-oxadiazoline

Inchi: InChI=1S/C7H12N2O2/c1-5-8-9(6(2)10)7(3,4)11-5/h1-4H3
InchiKey: TUTYXDDZVWGIMV-UHFFFAOYSA-N
Formula: C7H12N2O2
SMILES: CC(=O)N1N=C(C)OC1(C)C
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: 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=R116562&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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