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

Inchi: InChI=1S/C8H14N2O2/c1-5-7(11)10-8(3,4)12-6(2)9-10/h5H2,1-4H3
InchiKey: MQUJVBPTLJEHGL-UHFFFAOYSA-N
Formula: C8H14N2O2
SMILES: CCC(=O)N1N=C(C)OC1(C)C
Mol. weight [g/mol]: 170.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	1.325		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R116577&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.