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

Inchi: InChI=1S/C11H20N2O2/c1-5-9-12-13(10(14)6-2)11(7-3,8-4)15-9/h5-8H2,1-4H3
InchiKey: ZQZFXVFDDUZYLA-UHFFFAOYSA-N
Formula: C11H20N2O2
SMILES: CCC(=O)N1N=C(CC)OC1(CC)CC
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	2.495		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
rinpol	1360.00		NIST Webbook
rinpol	1360.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116557&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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