5,5-Pentamethylene-4-acetyl-1,3,4-oxadiazoline

Inchi: InChI=1S/C9H14N2O2/c1-8(12)11-9(13-7-10-11)5-3-2-4-6-9/h7H,2-6H2,1H3
InchiKey: SBZPNLOWXISGLR-UHFFFAOYSA-N
Formula: C9H14N2O2
SMILES: CC(=O)N1N=COC12CCCCC2
Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	1.469		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116715&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.