2-pentyl-4-methyoxazole

Inchi: InChI=1S/C9H15NO/c1-3-4-5-6-9-10-8(2)7-11-9/h7H,3-6H2,1-2H3
InchiKey: QPKLQTHGELMTTA-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: CCCCCc1nc(C)co1
Mol. weight [g/mol]: 153.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.51		Crippen Method
logp	2.716		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpol	1090.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R161458&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