2-pentyl-4,5-dimethyloxazole

Inchi: InChI=1S/C10H17NO/c1-4-5-6-7-10-11-8(2)9(3)12-10/h4-7H2,1-3H3
InchiKey: HLNGYNXFRKTMHQ-UHFFFAOYSA-N
Formula: C10H17NO
SMILES: CCCCCc1nc(C)c(C)o1
Mol. weight [g/mol]: 167.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.98		Crippen Method
logp	3.024		Crippen Method
mcvol	148.150	ml/mol	McGowan Method

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=R161438&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume