Oxazole, 5-ethyl-2-methyl-4-propyl

Inchi: InChI=1S/C9H15NO/c1-4-6-8-9(5-2)11-7(3)10-8/h4-6H2,1-3H3
InchiKey: UXLXRNTXKGMQEG-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: CCCc1nc(C)oc1CC
Mol. weight [g/mol]: 153.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.47		Crippen Method
logp	2.498		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpol	1079.00		NIST Webbook
ripol	1374.00		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=R61906&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
ripol: Polar retention indices