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

Other names: 2-ethyl-4-methyl-5-propyloxazole
Inchi: InChI=1S/C9H15NO/c1-4-6-8-7(3)10-9(5-2)11-8/h4-6H2,1-3H3
InchiKey: FDMDJAGBUGUESB-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: CCCc1oc(CC)nc1C
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
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1071.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1374.00		NIST Webbook

Sources

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=R46146&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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