Oxazole, 2,5-dimethyl-4-propyl

Other names: 4-n-propyl-2,5-dimethyloxazole
Inchi: InChI=1S/C8H13NO/c1-4-5-8-6(2)10-7(3)9-8/h4-5H2,1-3H3
InchiKey: GVCPWBGRQAPLQO-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: CCCc1nc(C)oc1C
Mol. weight [g/mol]: 139.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.14		Crippen Method
logp	2.244		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1319.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R61835&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

ripol: Polar retention indices