Oxazole, 2,4-dimethyl-5-propyl

Other names: 2,4-dimethyl-5-propyloxazole
Inchi: InChI=1S/C8H13NO/c1-4-5-8-6(2)9-7(3)10-8/h4-5H2,1-3H3
InchiKey: PSGAPKDEFJWSNU-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: CCCc1oc(C)nc1C
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
rinpol	989.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1319.00		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=R46128&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