Oxazole, 2-ethyl-5-methyl

Inchi: InChI=1S/C6H9NO/c1-3-6-7-4-5(2)8-6/h4H,3H2,1-2H3
InchiKey: ADIDFXCLFPHHLE-UHFFFAOYSA-N
Formula: C6H9NO
SMILES: CCc1ncc(C)o1
Mol. weight [g/mol]: 111.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.25		Crippen Method
logp	1.545		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
rinpol	820.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	851.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1204.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R46089&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