Oxazole, 2-ethyl-4-methyl

Inchi: InChI=1S/C6H9NO/c1-3-6-7-5(2)4-8-6/h4H,3H2,1-2H3
InchiKey: SRXOCFLMVTXDRQ-UHFFFAOYSA-N
Formula: C6H9NO
SMILES: CCc1nc(C)co1
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	818.00		NIST Webbook
rinpol	818.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1161.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1193.00		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=R46132&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