Oxazole, 5-ethyl-2-methyl

Other names: Oxazole, 2-methyl-5-ethyl
Inchi: InChI=1S/C6H9NO/c1-3-6-4-7-5(2)8-6/h4H,3H2,1-2H3
InchiKey: KVHQALCDTOJIBP-UHFFFAOYSA-N
Formula: C6H9NO
SMILES: CCc1cnc(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	818.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	855.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1210.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1222.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R46178&Units=SI
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

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