Oxazole, 4,5-diethyl

Inchi: InChI=1S/C7H11NO/c1-3-6-7(4-2)9-5-8-6/h5H,3-4H2,1-2H3
InchiKey: OCNQWGMIRHLWNN-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CCc1ncoc1CC
Mol. weight [g/mol]: 125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.58		Crippen Method
logp	1.799		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
rinpol	940.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R61853&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

Latest version available from: