Oxazole, 4-methyl-2-propyl

Inchi: InChI=1S/C7H11NO/c1-3-4-7-8-6(2)5-9-7/h5H,3-4H2,1-2H3
InchiKey: BUOGNIOVIYHMFO-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CCCc1nc(C)co1
Mol. weight [g/mol]: 125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.67		Crippen Method
logp	1.936		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
rinpol	901.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	901.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1229.00		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=R46196&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