Oxazole, 5-methyl-2-propyl

Inchi: InChI=1S/C7H11NO/c1-3-4-7-8-5-6(2)9-7/h5H,3-4H2,1-2H3
InchiKey: NZRDFBNIWMSPHP-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CCCc1ncc(C)o1
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	910.00		NIST Webbook
rinpol	910.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1247.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R61910&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