Oxazole, 5-ethyl-2-propyl

Inchi: InChI=1S/C8H13NO/c1-3-5-8-9-6-7(4-2)10-8/h6H,3-5H2,1-2H3
InchiKey: QQCWDOQKZRFUKY-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: CCCc1ncc(CC)o1
Mol. weight [g/mol]: 139.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.00		Crippen Method
logp	2.190		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
rinpol	1024.00		NIST Webbook
rinpol	1024.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1347.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R46203&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