Oxazole, 4-ethyl-5-propyl

Inchi:	InChI=1S/C8H13NO/c1-3-5-8-7(4-2)9-6-10-8/h6H,3-5H2,1-2H3
InchiKey:	AFLLKWKRNQXVTR-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	CCCc1ocnc1CC
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

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=R61871&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

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