

Oxazole, 2,5-dimethyl-4-propyl

Other names:	4-n-propyl-2,5-dimethyloxazole
Inchi:	InChI=1S/C8H13NO/c1-4-5-8-6(2)10-7(3)9-8/h4-5H2,1-3H3
InchiKey:	GVCPWBGRQAPLQO-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	CCCc1nc(C)oc1C
Mol. weight [g/mol]:	139.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.14		Crippen Method
logp	2.244		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1319.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R61835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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