Oxazole, 4-ethyl-2,5-dimethyl-

Other names:	2,5-Dimethyl-4-ethyloxazole
	4-ethyl-2,5-dimethyloxazole
Inchi:	InChI=1S/C7H11NO/c1-4-7-5(2)9-6(3)8-7/h4H2,1-3H3
InchiKey:	YZZBROGKUWYQOL-UHFFFAOYSA-N
Formula:	C7H11NO
SMILES:	CCc1nc(C)oc1C
Mol. weight [g/mol]:	125.17
CAS:	30408-61-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	1.854		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
rinpol	923.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook
ripol	1231.00		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1213.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30408618&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