

Oxazole, 5-ethyl-2,4-dimethyl

Other names:	2,4-dimethyl-5-ethyloxazole Oxazole, 2,4-dimethyl-5-ethyl
Inchi:	InChI=1S/C7H11NO/c1-4-7-5(2)8-6(3)9-7/h4H2,1-3H3
InchiKey:	XOOCKFZHDAFKNK-UHFFFAOYSA-N
Formula:	C7H11NO
SMILES:	CCc1oc(C)nc1C
Mol. weight [g/mol]:	125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	1.854		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
ripol	907.00		NIST Webbook
ripol	923.00		NIST Webbook
ripol	923.00		NIST Webbook
ripol	926.00		NIST Webbook
ripol	907.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1247.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1252.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R46114&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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