

Oxazole, 2,4-diethyl

Other names:	2,4-diethyloxazole
Inchi:	InChI=1S/C7H11NO/c1-3-6-5-9-7(4-2)8-6/h5H,3-4H2,1-2H3
InchiKey:	XIRWXQAIUBUNOH-UHFFFAOYSA-N
Formula:	C7H11NO
SMILES:	CCc1coc(CC)n1
Mol. weight [g/mol]:	125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.58		Crippen Method
logp	1.799		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	903.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1228.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R46100&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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