Oxazole, 2,4-dimethyl-

Other names: 2,4-Dimethyloxazole
Inchi: InChI=1S/C5H7NO/c1-4-3-7-5(2)6-4/h3H,1-2H3
InchiKey: PSOZJOZKEVZLKZ-UHFFFAOYSA-N
Formula: C5H7NO
SMILES: Cc1coc(C)n1
Mol. weight [g/mol]: 97.12
CAS: 7208-05-1

Physical Properties

Property code	Value	Unit	Source
ie	9.10	eV	NIST Webbook
ie	9.34	eV	NIST Webbook
log10ws	-5.92		Crippen Method
logp	1.291		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1087.00		NIST Webbook
tb	381.20	K	NIST Webbook

Sources

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=C7208051&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature

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