Oxazole, 2,5-dimethyl-

Other names: 2,5-dimethyloxazole
Inchi: InChI=1S/C5H7NO/c1-4-3-6-5(2)7-4/h3H,1-2H3
InchiKey: NSAUQTCATRWAJC-UHFFFAOYSA-N
Formula: C5H7NO
SMILES: Cc1cnc(C)o1
Mol. weight [g/mol]: 97.12
CAS: 23012-11-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	1.291		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
rinpol	765.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	730.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1133.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1145.00		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=C23012115&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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