

Oxazole, 4,5-dimethyl-

Other names:	4,5-Dimethyloxazole 5-Methyl-4-methyloxazole
Inchi:	InChI=1S/C5H7NO/c1-4-5(2)7-3-6-4/h3H,1-2H3
InchiKey:	YVORRVFKHZLJGZ-UHFFFAOYSA-N
Formula:	C5H7NO
SMILES:	Cc1ncoc1C
Mol. weight [g/mol]:	97.12
CAS:	20662-83-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	1.291		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
ripol	750.00		NIST Webbook
ripol	763.00		NIST Webbook
ripol	763.00		NIST Webbook
ripol	796.00		NIST Webbook
ripol	765.00		NIST Webbook
ripol	750.00		NIST Webbook
ripol	761.00		NIST Webbook
ripol	771.00		NIST Webbook
ripol	769.00		NIST Webbook
ripol	760.00		NIST Webbook
ripol	755.00		NIST Webbook
ripol	765.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1152.00		NIST Webbook

ripol	1139.00	NIST Webbook
ripol	1139.00	NIST Webbook
ripol	1139.00	NIST Webbook
ripol	1140.00	NIST Webbook
ripol	1141.00	NIST Webbook
ripol	1142.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C20662833&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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