4,5-Dimethyl-2-isopropyloxazole

Other names:	Oxazole, 4,5-dimethyl-2-(1-methylethyl)- 2-iso-Propyl-4,5-dimethyloxazole Oxazole, 2-isopropyl-4,5-dimethyl
Inchi:	InChI=1S/C8H13NO/c1-5(2)8-9-6(3)7(4)10-8/h5H,1-4H3
InchiKey:	OHMVVHYBMWXHSY-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	Cc1nc(C(C)C)oc1C
Mol. weight [g/mol]:	139.19
CAS:	19519-45-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.11		Crippen Method
logp	2.415		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
rinpol	938.00		NIST Webbook
rinpol	960.00		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1261.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C19519450&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