Oxazole, 4,5-dimethyl-2-(1-1-methylethyl)

Inchi: InChI=1S/C9H15NO/c1-6-7(2)11-8(10-6)9(3,4)5/h1-5H3
InchiKey: MUIYMEWBZZEDIG-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: Cc1nc(C(C)(C)C)oc1C
Mol. weight [g/mol]: 153.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	2.589		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
ripol	1249.00		NIST Webbook
ripol	1249.00		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=R410790&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
ripol: Polar retention indices

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