4,5-Dimethyl-2-isobutyloxazole

Other names:	Oxazole, 4,5-dimethyl-2-(2-methylpropyl)-
	2-iso-Butyl-4,5-dimethyloxazole
	2-Isobutyl-4,5-dimethyl-1,3-oxazole
	Oxazole, 4,5-dimethyl-2-isobutyl
	4,5-Dimethyl-2-(2-methylpropyl)-1,3-oxazole
Inchi:	InChI=1S/C9H15NO/c1-6(2)5-9-10-7(3)8(4)11-9/h6H,5H2,1-4H3
InchiKey:	SNRVAFQIIFPYDR-UHFFFAOYSA-N
Formula:	C9H15NO
SMILES:	Cc1nc(CC(C)C)oc1C
Mol. weight [g/mol]:	153.22
CAS:	26131-91-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.32		Crippen Method
logp	2.490		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpol	1044.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1330.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26131919&Units=SI
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

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