

2-Butyl-4,5-dimethyloxazole

Other names:	Oxazole, 2-butyl-4,5-dimethyl-
Inchi:	InChI=1S/C9H15NO/c1-4-5-6-9-10-7(2)8(3)11-9/h4-6H2,1-3H3
InchiKey:	VAGMYBQNOAXNOV-UHFFFAOYSA-N
Formula:	C9H15NO
SMILES:	CCCCc1nc(C)c(C)o1
Mol. weight [g/mol]:	153.22
CAS:	84027-97-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.56		Crippen Method
logp	2.634		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpol	1096.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C84027974&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

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