

Oxazole, 4-butyl-2,5-dimethyl

Other names:	2,5-dimethyl-4-butyloxazole
Inchi:	InChI=1S/C9H15NO/c1-4-5-6-9-7(2)11-8(3)10-9/h4-6H2,1-3H3
InchiKey:	MRXQRKKZDKCDSE-UHFFFAOYSA-N
Formula:	C9H15NO
SMILES:	CCCCc1nc(C)oc1C
Mol. weight [g/mol]:	153.23

Physical Properties

Property code	Value	Unit	Source
logp	2.634		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpol	1082.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1342.00		NIST Webbook
tb	454.16	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R161334&Units=SI

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

ripol: Polar retention indices
tb: Normal Boiling Point Temperature

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