

Oxazole, 4-butyl-2(5)-methyl

Other names:	4-n-butyl-2-methyloxazole
Inchi:	InChI=1S/C8H13NO/c1-3-4-5-8-6-10-7(2)9-8/h6H,3-5H2,1-2H3
InchiKey:	WLQJVRMHBOMLBM-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	CCCCc1coc(C)n1
Mol. weight [g/mol]:	139.20

Physical Properties

Property code	Value	Unit	Source
ie	8.92	eV	Cheméo Relay (1.0)
logp	2.326		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
rinpol	993.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1291.00		NIST Webbook
tb	438.63	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R161394&Units=SI
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):	

Legend

ie:	Ionization energy
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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<https://www.chemeo.com/cid/50-721-5/Oxazole-4-butyl-2-5-methyl.pdf>

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