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