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