

2,4-dimethyl-5-butyloxazole

Inchi: InChI=1S/C9H15NO/c1-4-5-6-9-7(2)10-8(3)11-9/h4-6H2,1-3H3
InchiKey: IXECKEKKCJBKQJ-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: CCCCc1oc(C)nc1C
Mol. weight [g/mol]: 153.22

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	1089.00		NIST Webbook
rinpol	1089.00		NIST Webbook

Sources

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=R161314&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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<https://www.chemeo.com/cid/43-877-1/2-4-dimethyl-5-butyloxazole.pdf>

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