

2-methyl-4-ethyl-5-propyloxazole

Inchi: InChI=1S/C9H15NO/c1-4-6-9-8(5-2)10-7(3)11-9/h4-6H2,1-3H3
InchiKey: OJFZPFCEFJXLIK-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: CCCc1oc(C)nc1CC
Mol. weight [g/mol]: 153.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.47		Crippen Method
logp	2.498		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpole	1067.00		NIST Webbook
rinpole	1067.00		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=R161403&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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/34-601-6/2-methyl-4-ethyl-5-propyloxazole.pdf>

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