2-iso-Butyl-4-ethyl-5-methyloxazole

Other names: 2-iso-Butyl-4-ethyl-5-methyloxazole
Oxazole, 4-ethyl-2-isobutyl-5-methyl
Inchi: InChI=1S/C10H17NO/c1-5-9-8(4)12-10(11-9)6-7(2)3/h7H,5-6H2,1-4H3
InchiKey: KGIIOPAYOWPZLL-UHFFFAOYSA-N
Formula: C10H17NO
SMILES: CCc1nc(CC(C)C)oc1C
Mol. weight [g/mol]: 167.25

Physical Properties

Property code	Value	Unit	Source
logp	2.744		Crippen Method
mcvol	148.150	ml/mol	McGowan Method
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
ripol	1359.00		NIST Webbook

Sources

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=U285056&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices