

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

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