

2-iso-Propyl-4-ethyl-5-methyloxazole

Other names:	Oxazole, 4-ethyl-2-isopropyl-5-methyl
Inchi:	InChI=1S/C9H15NO/c1-5-8-7(4)11-9(10-8)6(2)3/h6H,5H2,1-4H3
InchiKey:	SGEREWZCOUDFEM-UHFFFAOYSA-N
Formula:	C9H15NO
SMILES:	CCc1nc(C(C)C)oc1C
Mol. weight [g/mol]:	153.22
CAS:	84027-96-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.43		Crippen Method
logp	2.669		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpol	1021.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1279.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84027963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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