

2-butyl-4,5-diethyloxazole

Inchi:	InChI=1S/C11H19NO/c1-4-7-8-11-12-9(5-2)10(6-3)13-11/h4-8H2,1-3H3
InchiKey:	LVIUUUNWXOKYDD-UHFFFAOYSA-N
Formula:	C11H19NO
SMILES:	CCCCc1nc(CC)c(CC)o1
Mol. weight [g/mol]:	181.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.22		Crippen Method
logp	3.142		Crippen Method
mcvol	162.240	ml/mol	McGowan Method
rinsol	1292.00		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=R161349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/43-734-9/2-butyl-4-5-diethyloxazole.pdf>

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