

2,4-Diethyl-5-methyloxazole

Other names:	Oxazole, 2,4-diethyl-5-methyl
Inchi:	InChI=1S/C8H13NO/c1-4-7-6(3)10-8(5-2)9-7/h4-5H2,1-3H3
InchiKey:	PEVDCYWBTUDNKS-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	CCc1nc(CC)c(C)o1
Mol. weight [g/mol]:	139.19
CAS:	84027-88-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.05		Crippen Method
logp	2.108		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
ripol	1274.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C84027883&Units=SI

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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