

5-Ethyl-5-methyl-4-propionyl-1,3,4-oxadiazoline

Inchi:	InChI=1S/C8H14N2O2/c1-4-7(11)10-8(3,5-2)12-6-9-10/h6H,4-5H2,1-3H3
InchiKey:	MZEUPXHNPADRNY-UHFFFAOYSA-N
Formula:	C8H14N2O2
SMILES:	CCC(=O)N1N=COC1(C)CC
Mol. weight [g/mol]:	170.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	1.325		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
rinsol	1130.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R116780&Units=SI

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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