

1-Phenyl-3-acetoxy-4-methyl-2-pyrazoline

Inchi:	InChI=1S/C12H14N2O2/c1-9-8-14(11-6-4-3-5-7-11)13-12(9)16-10(2)15/h3-7,9H,8H2,1-2
InchiKey:	XPGTVRIUDBONFO-UHFFFAOYSA-N
Formula:	C12H14N2O2
SMILES:	CC(=O)OC1=NN(c2ccccc2)CC1C
Mol. weight [g/mol]:	218.25
CAS:	2748-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	2.019		Crippen Method
mcvol	168.420	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2748223&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

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<https://www.chemeo.com/cid/112-955-7/1-Phenyl-3-acetoxy-4-methyl-2-pyrazoline.pdf>

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