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/ci990307l
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