1-Phenyl-3-acetoxy-2-pyrazoline

Inchi: InChI=1S/C11H12N2O2/c1-9(14)15-11-7-8-13(12-11)10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey: KEKBLIAQVPGFMT-UHFFFAOYSA-N
Formula: C11H12N2O2
SMILES: CC(=O)OC1=NN(c2ccccc2)CC1
Mol. weight [g/mol]: 204.23
CAS: 2748-21-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.773		Crippen Method
mcvol	154.330	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=C2748212&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