1-Phenyl-2-acetyl-4-methyl-3-pyrazolidone

Other names: 2-acetyl-4-methyl-1-phenylpyrazolidin-3-one
Inchi: InChI=1S/C12H14N2O2/c1-9-8-13(11-6-4-3-5-7-11)14(10(2)15)12(9)16/h3-7,9H,8H2,1-2
InchiKey: BPNPRBBKUKZUCD-UHFFFAOYSA-N
Formula: C12H14N2O2
SMILES: CC(=O)N1C(=O)C(C)CN1c1ccccc1
Mol. weight [g/mol]: 218.25
CAS: 2655-48-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.82		Crippen Method
logp	1.433		Crippen Method
mcvol	168.420	ml/mol	McGowan Method

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=C2655483&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume