1-Phenyl-2-acetyl-3-pyrazolidone

Inchi: InChI=1S/C11H12N2O2/c1-9(14)13-11(15)7-8-12(13)10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey: GCYDZZBQYRCILB-UHFFFAOYSA-N
Formula: C11H12N2O2
SMILES: CC(=O)N1C(=O)CCN1c1ccccc1
Mol. weight [g/mol]: 204.23
CAS: 2655-46-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.187		Crippen Method
mcvol	154.330	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=C2655461&Units=SI

Legend

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