

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/48-698-5/1-Phenyl-2-acetyl-3-pyrazolidone.pdf>

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