2-Pyrrolidinone, 1-(1-benzoylethyl)

Inchi: InChI=1S/C13H15NO2/c1-10(14-9-5-8-12(14)15)13(16)11-6-3-2-4-7-11/h2-4,6-7,10H,5,8
InchiKey: LZFDBIIMVDBINR-UHFFFAOYSA-N
Formula: C13H15NO2
SMILES: CC(C(=O)c1ccccc1)N1CCCC1=O
Mol. weight [g/mol]: 217.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	1.880		Crippen Method
mcvol	172.530	ml/mol	McGowan Method
rinpol	1820.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R404285&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
rinpol: Non-polar retention indices