2-Pyrrolidinone, 1-(1-(4-methylbenzoyl)ethyl)

Other names: 4'-Methyl-«alpha»-pyrrolidinopropiophenone-M (oxo-)
Inchi: InChI=1S/C14H17NO2/c1-10-5-7-12(8-6-10)14(17)11(2)15-9-3-4-13(15)16/h5-8,11H,3-4
InchiKey: MQHIRDVFNSYBCC-UHFFFAOYSA-N
Formula: C14H17NO2
SMILES: Cc1ccc(C(=O)C(C)N2CCCC2=O)cc1
Mol. weight [g/mol]: 231.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.189		Crippen Method
mcvol	186.620	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook

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=R284214&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices