1-(4-Methylphenyl)-2-(pyrrolidin-2-one-1-yl)-1-buta

Other names: 4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (oxo-)
Inchi: InChI=1S/C15H19NO2/c1-3-13(16-10-4-5-14(16)17)15(18)12-8-6-11(2)7-9-12/h6-9,13H,
InchiKey: CDOWAWOYIGHBQS-UHFFFAOYSA-N
Formula: C15H19NO2
SMILES: CCC(C(=O)c1ccc(C)cc1)N1CCCC1=O
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	2.579		Crippen Method
mcvol	200.710	ml/mol	McGowan Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook

Sources

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=U360387&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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