4-[(2-Pyrrolidin-1-yl)-1-butanoyl]benzoic acid, methyl ester

Other names: 4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-) methyl
Inchi: InChI=1S/C16H21NO3/c1-3-14(17-10-4-5-11-17)15(18)12-6-8-13(9-7-12)16(19)20-2/h6-9
InchiKey: KZJAYAMSDYKHIW-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCC(C(=O)c1ccc(C(=O)OC)cc1)N1CCCC1
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.530		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		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=U360388&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