Pyrrolidin-2-one, 1-[1-(4-carbomethoxyphenyl)butan-1-ol-2-yl]-

Other names: 4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-oxo-dihydro-) methyl
Inchi: InChI=1S/C16H21NO4/c1-3-13(17-10-4-5-14(17)18)15(19)11-6-8-12(9-7-11)16(20)21-2/h
InchiKey: BULBLXXKCKVDBY-UHFFFAOYSA-N
Formula: C16H21NO4
SMILES: CCC(C(O)c1ccc(C(=O)OC)cc1)N1CCCC1=O
Mol. weight [g/mol]: 291.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.908		Crippen Method
mcvol	226.540	ml/mol	McGowan Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		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=U360390&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