4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-oxo-) methyl

Inchi: InChI=1S/C16H19NO4/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: XSTBXKHJQWTRJY-UHFFFAOYSA-N
Formula: C16H19NO4
SMILES: CCC(C(=O)c1ccc(C(=O)OC)cc1)N1CCCC1=O
Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.057		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R417360&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.