4'-Ethoxycarbonyl-«alpha»-pyrrolidinohexanophe

Other names: R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone-M (carboxy-), ethylated
Inchi: InChI=1S/C19H27NO3/c1-3-5-8-17(20-13-6-7-14-20)18(21)15-9-11-16(12-10-15)19(22)2
InchiKey: FDNPZAZPXFGMPZ-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CCCCC(C(=O)c1ccc(C(=O)OCC)cc1)N1CCCC1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	3.701		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U314301&Units=SI
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

Legend

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