4'-Ethoxycarbonyl-«alpha»-(2-oxopyrrolidino)hex

Other names: R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone-M (oxo-carboxy-), ethylated
Inchi: InChI=1S/C19H25NO4/c1-3-5-7-16(20-13-6-8-17(20)21)18(22)14-9-11-15(12-10-14)19(2
InchiKey: QEASLYZJXRLGDJ-UHFFFAOYSA-N
Formula: C19H25NO4
SMILES: CCCCC(C(=O)c1ccc(C(=O)OCC)cc1)N1CCCC1=O
Mol. weight [g/mol]: 331.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	3.227		Crippen Method
mcvol	264.510	ml/mol	McGowan Method
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U314302&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