R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone (oxo-carboxy-HO-alkyl-): ethylated

Inchi: InChI=1S/C19H25NO5/c1-3-6-15(21)17(20-12-5-7-16(20)22)18(23)13-8-10-14(11-9-13)1

InchiKey: XHKUEFGNSDNKAC-UHFFFAOYSA-N

Formula: C19H25NO5

SMILES: CCCC(O)C(C(=O)c1ccc(C(=O)OCC)cc1)N1CCCC1=O

Mol. weight [g/mol]: 347.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	2.198		Crippen Method
mcvol	270.380	ml/mol	McGowan Method
rinpol	2640.00		NIST Webbook
rinpol	2665.00		NIST Webbook
rinpol	2640.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290883&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