R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone (HO-alkyl-) isomer-1, AC

Inchi: InChI=1S/C19H27NO3/c1-4-7-17(23-15(3)21)18(20-12-5-6-13-20)19(22)16-10-8-14(2)9-
InchiKey: YKXCOVTVNNNNMY-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CCCC(OC(C)=O)C(C(=O)c1ccc(C)cc1)N1CCCC1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.374		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2245.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290838&Units=SI

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.