R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone (di-HO-), 2AC

Inchi: InChI=1S/C21H29NO5/c1-5-6-9-18(22-10-7-8-11-22)21(25)17-13-19(26-15(3)23)14(2)12

InchiKey: JUFGHRHVZXFOBJ-UHFFFAOYSA-N

Formula: C21H29NO5

SMILES: CCCCC(C(=O)c1cc(OC(C)=O)c(C)cc1OC(C)=O)N1CCCC1

Mol. weight [g/mol]: 375.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	3.683		Crippen Method
mcvol	298.560	ml/mol	McGowan Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2600.00		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=R290818&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