R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone (oxo-HO-toluol-), AC

Inchi: InChI=1S/C19H25NO4/c1-4-5-7-16(20-11-6-8-18(20)22)19(23)15-10-9-13(2)17(12-15)24

InchiKey: RNFXXPRUCLOJKK-UHFFFAOYSA-N

Formula: C19H25NO4

SMILES: CCCCC(C(=O)c1ccc(C)c(OC(C)=O)c1)N1CCCC1=O

Mol. weight [g/mol]: 331.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	3.284		Crippen Method
mcvol	264.510	ml/mol	McGowan Method
rinpol	2515.00		NIST Webbook

Sources

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=R290907&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices