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

Inchi: InChI=1S/C19H27NO3/c1-4-5-8-17(20-11-6-7-12-20)19(22)16-10-9-14(2)18(13-16)23-15

InchiKey: SONAKEOUMLGFED-UHFFFAOYSA-N

Formula: C19H27NO3

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

Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	3.758		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290843&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.