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

Inchi: InChI=1S/C19H25NO4/c1-4-6-16(24-14(3)21)18(20-12-5-7-17(20)22)19(23)15-10-8-13(2

InchiKey: IGKPEQMXXZQEIF-UHFFFAOYSA-N

Formula: C19H25NO4

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

Mol. weight [g/mol]: 331.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	2.901		Crippen Method
mcvol	264.510	ml/mol	McGowan Method
rinpol	2425.00		NIST Webbook
rinpol	2425.00		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=R290898&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.