

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

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: JUFGRHVZXFQBJ-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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R290818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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