R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone (carboxy-HO-alkyl-), ethylated

Inchi: InChI=1S/C19H27NO4/c1-3-7-16(21)17(20-12-5-6-13-20)18(22)14-8-10-15(11-9-14)19(2

InchiKey: RUYBJGPDIGJWKP-UHFFFAOYSA-N

Formula: C19H27NO4

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

Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.09		Crippen Method
logp	2.671		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
rinpol	2535.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2535.00		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=R290803&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

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