

4'-Ethoxycarbonyl-«alpha»-pyrrolidinohexanophene

Other names:	R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone-M (carboxy-), ethylated
Inchi:	InChI=1S/C19H27NO3/c1-3-5-8-17(20-13-6-7-14-20)18(21)15-9-11-16(12-10-15)19(22)2
InchiKey:	FDNPZAZPXFEMPZ-UHFFFAOYSA-N
Formula:	C19H27NO3
SMILES:	CCCCC(C(=O)c1ccc(C(=O)OCC)cc1)N1CCCC1
Mol. weight [g/mol]:	317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	3.701		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U314301&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

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