4'-Methyl-«alpha»-pyrrolidinopropiophenone-M (carboxy-), ethylated

Inchi: InChI=1S/C16H21NO3/c1-3-20-16(19)14-8-6-13(7-9-14)15(18)12(2)17-10-4-5-11-17/h6-9
InchiKey: OPBPPIZVTYWETI-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCOC(=O)c1ccc(C(=O)C(C)N2CCCC2)cc1
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.530		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R284209&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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