R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenon (desmethyl-), ethylated

Other names: Pyrrolidine, 1-(1-(4-ethoxybenzoyl)ethyl)
Inchi: InChI=1S/C15H21NO2/c1-3-18-14-8-6-13(7-9-14)15(17)12(2)16-10-4-5-11-16/h6-9,12H,
InchiKey: DJKDTLFRWPMBBA-UHFFFAOYSA-N
Formula: C15H21NO2
SMILES: CCOc1ccc(C(=O)C(C)N2CCCC2)cc1
Mol. weight [g/mol]: 247.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.752		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290581&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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