R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenon (desmethyl-3-methoxy-) ethylated

Other names: R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinopropiophenone-M (desmethylene-3-methoxy-), ethylated

Inchi: InChI=1S/C16H23NO3/c1-4-20-14-8-7-13(11-15(14)19-3)16(18)12(2)17-9-5-6-10-17/h7-8

InchiKey: NORMSIYETVUKMK-UHFFFAOYSA-N

Formula: C16H23NO3

SMILES: CCOc1ccc(C(=O)C(C)N2CCCC2)cc1OC

Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.761		Crippen Method
mcvol	224.970	ml/mol	McGowan Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290610&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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