R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenon (desmethyl-3HO-), 2ET

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

Inchi: InChI=1S/C17H25NO3/c1-4-20-15-9-8-14(12-16(15)21-5-2)17(19)13(3)18-10-6-7-11-18/h

InchiKey: DVJPWRRCEUOMPF-UHFFFAOYSA-N

Formula: C17H25NO3

SMILES: CCOc1ccc(C(=O)C(C)N2CCCC2)cc1OCC

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	3.151		Crippen Method
mcvol	239.060	ml/mol	McGowan Method
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2165.00		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=R290605&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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