

R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenone

Inchi:
(Oxo-)

InChI=1S/C14H17NO3/c1-10(15-9-3-4-13(15)16)14(17)11-5-7-12(18-2)8-6-11/h5-8,10H,

InchiKey:

RTPIZHDULKIEET-UHFFFAOYSA-N

Formula:

C14H17NO3

SMILES:

COc1ccc(C(=O)C(C)N2CCCC2=O)cc1

Mol. weight [g/mol]:

247.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.889		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
rinpol	2120.00		NIST Webbook
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Sources

Crippen Method:

https://www.cheméo.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=R290645&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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