

MOPPP

Other names: R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenone
Inchi: InChI=1S/C14H19NO2/c1-11(15-9-3-4-10-15)14(16)12-5-7-13(17-2)8-6-12/h5-8,11H,3-4
InchiKey: QJWOQBGBEFNYKB-UHFFFAOYSA-N
Formula: C14H19NO2
SMILES: COc1ccc(C(=O)C(C)N2CCCC2)cc1
Mol. weight [g/mol]: 233.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	2.362		Crippen Method
mcvol	190.920	ml/mol	McGowan Method
rinpola	1705.00		NIST Webbook
rinpola	1705.00		NIST Webbook

Sources

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=U386337&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/121-077-2/MOPPP.pdf>

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