

MDPPP

Other names:

3',4'-Methylenedioxy- α -pyrrolidinopropiophenone
R,S-3',4'-methylenedioxy- α -pyrrolidinopropiophenone

Inchi: InChI=1S/C14H17NO3/c1-10(15-6-2-3-7-15)14(16)11-4-5-12-13(8-11)18-9-17-12/h4-5,8,**InchiKey:** NIYQOTCYXGXMPI-UHFFFAOYSA-N**Formula:** C14H17NO3**SMILES:** CC(C(=O)c1ccc2c(c1)OCO2)N1CCCC1**Mol. weight [g/mol]:** 247.29**CAS:** 24698-57-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	2.082		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C24698575&Units=SI>**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

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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