MDPPP

Other names:	3',4'-Methylenedioxy-a-pyrrolidinopropiophenone
	R,S-3',4'-methylenedioxy-«alpha»-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/ci990307l
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