R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinoprop (oxo-)

Inchi: InChI=1S/C14H15NO4/c1-9(15-6-2-3-13(15)16)14(17)10-4-5-11-12(7-10)19-8-18-11/h4-5
InchiKey: PMTXPXOBUUDUAJ-UHFFFAOYSA-N
Formula: C14H15NO4
SMILES: CC(C(=O)c1ccc2c(c1)OCO2)N1CCCC1=O
Mol. weight [g/mol]: 261.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	1.609		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290754&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.