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

InChI: InChI=1S/C17H23NO4/c1-4-21-14-9-8-13(11-15(14)22-5-2)17(20)12(3)18-10-6-7-16(18)

InChIKey: UAOWYDHUKWDZFV-UHFFFAOYSA-N

Formula: C17H23NO4

SMILES: CCOc1ccc(C(=O)C(C)N2CCCC2=O)cc1OCC

Mol. weight [g/mol]: 305.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.678		Crippen Method
mcvol	240.630	ml/mol	McGowan Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290734&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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.