Piperazine, 1-phenyl-4-(2,3-diacetoxypropyl)

Inchi: InChI=1S/C17H24N2O4/c1-14(20)22-13-17(23-15(2)21)12-18-8-10-19(11-9-18)16-6-4-3-
InchiKey: HVMNGGLXSZZRLK-UHFFFAOYSA-N
Formula: C17H24N2O4
SMILES: CC(=O)OCC(CN1CCN(c2ccccc2)CC1)OC(C)=O
Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.45		Crippen Method
logp	1.303		Crippen Method
mcvol	250.610	ml/mol	McGowan Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R404483&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

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