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

Inchi: InChI=1S/C19H26N2O6/c1-14(22)25-13-19(27-16(3)24)12-20-8-10-21(11-9-20)17-4-6-18

InchiKey: YFXFGKIUERQJPK-UHFFFAOYSA-N

Formula: C19H26N2O6

SMILES: CC(=O)OCC(CN1CCN(c2ccc(OC(C)=O)cc2)CC1)OC(C)=O

Mol. weight [g/mol]: 378.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	1.229		Crippen Method
mcvol	286.230	ml/mol	McGowan Method
rinpol	2675.00		NIST Webbook
rinpol	2675.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R404458&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.