(1R,9S)-1-Acetoxy-N-acetyl-1,9-dihydro-anhydron

Inchi: InChI=1S/C25H27NO10/c1-13(27)26-9-8-15-10-18-22(35-12-34-18)23(33-5)20(15)25(26
InchiKey: JYLSYDBZXRABOF-RUZDIDTESA-N
Formula: C25H27NO10
SMILES: COc1ccc(CC2(OC(C)=O)c3c(cc4c(c3OC)OCO4)CCN2C(C)=O)c(C(=O)O)c1OC
Mol. weight [g/mol]: 501.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	2.502		Crippen Method
mcvol	349.650	ml/mol	McGowan Method
rinpol	3848.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R330733&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