Cytosine arabinoside, acetyl methyl derivative

Inchi: InChI=1S/C18H23N3O9/c1-9(22)20(5)14-6-7-21(18(26)19-14)17-16(30-12(4)25)15(29-11
InchiKey: CTSFZJISMPDJNX-YJNKEBTESA-N
Formula: C18H23N3O9
SMILES: CC(=O)OC1COC(n2ccc(N(C)C(C)=O)nc2=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 425.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.15		Crippen Method
logp	-0.450		Crippen Method
mcvol	295.430	ml/mol	McGowan Method
rinpol	2720.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R245779&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices