Cytidine, acetyl methyl derivative

Inchi: InChI=1S/C17H21N3O9/c1-8(21)19(5)12-6-7-20(17(25)18-12)15-13(26-9(2)22)14(27-10(
InchiKey: NQEIBWIRZUSAEO-FJBKBRRZSA-N
Formula: C17H21N3O9
SMILES: CC(=O)OC1OC(n2ccc(N(C)C(C)=O)nc2=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 411.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.23		Crippen Method
logp	-0.493		Crippen Method
mcvol	281.340	ml/mol	McGowan Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R245719&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.