3',5'-Diacetylthymidine

Other names:	Thymidine, 3',5'-diacetate
	Thymidine, 3',5'-bis-O-acetyl
Inchi:	InChI=1S/C14H18N2O7/c1-7-5-16(14(20)15-13(7)19)12-4-10(22-9(3)18)11(23-12)6-21-8
InchiKey:	RGVBNBFNSBMXID-UHFFFAOYSA-N
Formula:	C14H18N2O7
SMILES:	CC(=O)OCC1OC(n2cc(C)c(=O)[nH]c2=O)CC1OC(C)=O
Mol. weight [g/mol]:	326.30
CAS:	6979-97-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.59		Crippen Method
logp	-0.855		Crippen Method
mcvol	225.950	ml/mol	McGowan Method
rinpol	2439.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6979971&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

Latest version available from: