

# Thymidine, 3',5'-bis(trifluoroacetate)

<b>Other names:</b>	O-3',5'-Bis(trifluoroacetyl)thymidine Thymidine, 3',5'-bis-O-TFA
<b>Inchi:</b>	InChI=1S/C14H12F6N2O7/c1-5-3-22(12(26)21-9(5)23)8-2-6(29-11(25)14(18,19)20)7(28
<b>InchiKey:</b>	XOTHCHOYOROZPJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H12F6N2O7
<b>SMILES:</b>	<chem>Cc1cn(C2CC(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)O2)c(=O)nc1O</chem>
<b>Mol. weight [g/mol]:</b>	434.24
<b>CAS:</b>	18354-10-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	1.124		Crippen Method
mcvol	236.570	ml/mol	McGowan Method
rinpol	2053.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2032.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C18354104&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18354104&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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