

# 1-(5',6'-dihydroxyhexyl)-3,7-dimethylxanthine, O-TFA

Inchi:	InChI=1S/C17H18F6N4O6/c1-25-8-24-11-10(25)12(28)27(15(31)26(11)2)6-4-3-5-9(33-1
InchiKey:	YUOVLRLUYXTZLQJ-UHFFFAOYSA-N
Formula:	C17H18F6N4O6
SMILES:	Cn1cnc2c1c(=O)n(CCCCC(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F)c(=O)n2C
Mol. weight [g/mol]:	488.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.23		Crippen Method
logp	1.184		Crippen Method
mcvol	288.630	ml/mol	McGowan Method
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R155047&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R155047&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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