

# threo-1-(4',5'-dihydroxyhexyl)-3,7-dimethylxanthine-O-TFA

InChI:  
InChIKey:

InChI=1S/C17H18F6N4O6/c1-8(32-13(29)16(18,19)20)9(33-14(30)17(21,22)23)5-4-6-27

IKPRVZPOMULNJV-IUCAKERBSA-N

Formula:

C17H18F6N4O6

SMILES:

CC(OC(=O)C(F)(F)F)C(CCCn1c(=O)c2c(ncn2C)n(C)c1=O)OC(=O)C(F)(F)F

Mol. weight [g/mol]:

488.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.35		Crippen Method
logp	1.182		Crippen Method
mcvol	288.630	ml/mol	McGowan Method
rinpol	2259.00		NIST Webbook

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R155092&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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