erythro-1-(4',5'-dihydroxyhexyl)-3,7-dimethylxanth O-TFA

Inchi: InChI=1S/C17H18F6N4O6/c1-8(32-13(29)16(18,19)20)9(33-14(30)17(21,22)23)5-4-6-27
InchiKey: IKPRVZPOMULNJV-DTWKUNHWSA-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	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R155087&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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