1-(6'-hydroxyhexyl)-3-methyl-7-propylxanthine, O-TFA

Inchi: InChI=1S/C17H23F3N4O4/c1-3-8-23-11-21-13-12(23)14(25)24(16(27)22(13)2)9-6-4-5-7-

InchiKey: WPJYXKGVJKQNTC-UHFFFAOYSA-N

Formula: C17H23F3N4O4

SMILES: CCCn1cnc2c1c(=O)n(CCCCCCOC(=O)C(F)(F)F)c(=O)n2C

Mol. weight [g/mol]: 404.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	1.973		Crippen Method
mcvol	275.880	ml/mol	McGowan Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook

Sources

Crippen Method: 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=R155067&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.