Xanthine, 1-(5'-hydroxyhexyl)-3-methyl-7-propyl, TFA

Inchi: InChI=1S/C17H23F3N4O4/c1-4-8-23-13-12(22(3)10-21-13)14(25)24(16(23)27)9-6-5-7-11
InchiKey: ZRXSFVYUNMDMTC-UHFFFAOYSA-N
Formula: C17H23F3N4O4
SMILES: CCCn1c(=O)n(CCCCC(C)OC(=O)C(F)(F)F)c(=O)c2c1ncn2C
Mol. weight [g/mol]: 404.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.26		Crippen Method
logp	1.971		Crippen Method
mcvol	275.880	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R146137&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.