Xanthine, 1-(5'-hydroxyhexyl)-3,7-dimethyl, TMS

Inchi: InChI=1S/C16H28N4O3Si/c1-12(23-24(4,5)6)9-7-8-10-20-15(21)13-14(17-11-18(13)2)19

InchiKey: GGVBURBTDDKMTI-UHFFFAOYSA-N

Formula: C16H28N4O3Si

SMILES: CC(CCCCn1c(=O)c2c(ncn2C)n(C)c1=O)O[Si](C)(C)C

Mol. weight [g/mol]: 352.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	1.844		Crippen Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R146117&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices