

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

Inchi:	InChI=1S/C18H32N4O3Si/c1-7-11-21-16-15(20(3)13-19-16)17(23)22(18(21)24)12-9-8-10
InchiKey:	OPAHZSPAXVXGMG-UHFFFAOYSA-N
Formula:	C18H32N4O3Si
SMILES:	CCCN1c(=O)n(CCCCC(C)O[Si](C)(C)C)c(=O)c2c1ncn2C
Mol. weight [g/mol]:	380.56

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	2.717		Crippen Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R146142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R146142&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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