Tris(trimethylsilyl) 5-nitrobarbiturate

Other names:	2,4,6-Tris(trimethylsilyloxy)-5-nitropyrimidine
	Tris(trimethylsilyl) diliturate
	Pyrimidine, 2,4,6-trihydroxy-5-nitro, TMS
Inchi:	InChI=1S/C13H27N3O5Si3/c1-22(2,3)19-11-10(16(17)18)12(20-23(4,5)6)15-13(14-11)21
InchiKey:	VENIUGMHRAWOKE-UHFFFAOYSA-N
Formula:	C13H27N3O5Si3
SMILES:	C[Si](C)(C)Oc1nc(O[Si](C)(C)C)c([N+](=O)[O-])c(O[Si](C)(C)C)n1
Mol. weight [g/mol]:	389.63

Physical Properties

Property code	Value	Unit	Source
log10ws	1.32		Crippen Method
logp	4.026		Crippen Method
rinpol	1821.00		NIST Webbook
rinpol	1806.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373188&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
rinpol:	Non-polar retention indices

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