

Pyrimidine, 2,4,6-tris[(trimethylsilyl)oxy]-

Other names:	Pyrimidine, 2,4,6-tris(trimethylsiloxy)- 2,4,6-Tris[(trimethylsilyl)oxy]pyrimidine Pyrimidine, 2,4,6-trihydroxy, (tris-TMS)- Barbituric acid, TMS Pyrimidine, 2,4,6-trihydroxy, TMS
Inchi:	InChI=1S/C13H28N2O3Si3/c1-19(2,3)16-11-10-12(17-20(4,5)6)15-13(14-11)18-21(7,8)9
InchiKey:	MTDRSUCYKPIFHV-UHFFFAOYSA-N
Formula:	C13H28N2O3Si3
SMILES:	<chem>C[Si](C)(C)Oc1cc(O[Si](C)(C)C)nc(O[Si](C)(C)C)n1</chem>
Mol. weight [g/mol]:	344.63
CAS:	31111-39-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.97		Crippen Method
logp	4.118		Crippen Method
rinpol	1592.00		NIST Webbook
rinpol	1600.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31111394&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
rinpol:	Non-polar retention indices

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