

5-Hydroxymethylcytosine, TMS

Other names:	Pyrimidine, 4-amino-2-hydroxy-5-hydroxymethyl, TMS
Inchi:	InChI=1S/C14H31N3O2Si3/c1-20(2,3)17-13-12(11-18-21(4,5)6)10-15-14(16-13)19-22(7,
InchiKey:	OBAAESGOHWDQMG-UHFFFAOYSA-N
Formula:	C14H31N3O2Si3
SMILES:	C[Si](C)(C)Nc1nc(O[Si](C)(C)C)ncc1CO[Si](C)(C)C
Mol. weight [g/mol]:	357.67

Physical Properties

Property code	Value	Unit	Source
log10ws	1.82		Crippen Method
logp	4.289		Crippen Method
rinsol	1750.00		NIST Webbook
rinsol	1752.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R93832&Units=SI

Legend

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

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