

Pyrimidine, 6-amino-4-hydroxy-5-hydroxyacetamino, TMS

Inchi:	InChI=1S/C15H32N4O3Si3/c1-23(2,3)19-14-13(18-12(20)10-21-24(4,5)6)15(17-11-16-14
InchiKey:	NJPOJAYGCIFQHW-UHFFFAOYSA-N
Formula:	C15H32N4O3Si3
SMILES:	C[Si](C)(C)Nc1ncnc(O[Si](C)(C)C)c1N=C(O)CO[Si](C)(C)C
Mol. weight [g/mol]:	400.70

Physical Properties

Property code	Value	Unit	Source
log10ws	2.31		Crippen Method
logp	4.377		Crippen Method
rinpol	2019.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387061&Units=SI

Legend

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

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