

5-Pyrimidinecarboxylic acid, 2,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	Pyrimidin-5-carboxylic acid, 2,4-dihydroxy, TMS
Inchi:	InChI=1S/C14H28N2O4Si3/c1-21(2,3)18-12-11(13(17)19-22(4,5)6)10-15-14(16-12)20-23
InchiKey:	XIVCUMXZIQOLKK-UHFFFAOYSA-N
Formula:	C14H28N2O4Si3
SMILES:	C[Si](C)(C)OC(=O)c1cnc(O[Si](C)(C)C)nc1O[Si](C)(C)C
Mol. weight [g/mol]:	372.64
CAS:	56804-96-7

Physical Properties

Property code	Value	Unit	Source
log10ws	1.85		Crippen Method
logp	3.896		Crippen Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		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=C56804967&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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