1-Methyladenine riboside, TMS

Inchi: InChI=1S/C23H47N5O4Si4/c1-27-15-25-21(26-33(2,3)4)18-22(27)28(16-24-18)23-20(32
InchiKey: YZANXFRGIUHCLY-SBGJYJENSA-N
Formula: C23H47N5O4Si4
SMILES: Cn1cnc(=N[Si](C)(C)C)c2ncn(C3OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C3O[Si](C)(C)C)c21
Mol. weight [g/mol]: 569.99

Physical Properties

Property code	Value	Unit	Source
log10ws	0.88		Crippen Method
logp	4.694		Crippen Method
rinpol	2760.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R93462&Units=SI

Legend

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