adenosine-3'-monophosphate, TMS

Inchi: InChI=1S/C25H54N5O6PSi5/c1-38(2,3)29-23-20-24(27-17-26-23)30(18-28-20)25-21(34-
InchiKey: LBUJHLOVLBSSMK-ODZZBHCRSA-N
Formula: C25H54N5O6PSi5
SMILES: C[Si](C)(C)Nc1ncnc2c1ncn2C1OC(CO[Si](C)(C)C)C(P(=O)(O[Si](C)(C)C)O[Si](C)(C)C)C
Mol. weight [g/mol]: 692.13

Physical Properties

Property code	Value	Unit	Source
log10ws	1.39		Crippen Method
logp	7.307		Crippen Method
rinpol	3028.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R485506&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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