6-methyl adenine, TMS

Inchi: InChI=1S/C12H23N5Si2/c1-9-15-11-10(17(9)19(5,6)7)12(14-8-13-11)16-18(2,3)4/h8H,1-
InchiKey: NFXMWMHXGYLTKC-UHFFFAOYSA-N
Formula: C12H23N5Si2
SMILES: Cc1nc2ncnc(N[Si](C)(C)C)c2n1[Si](C)(C)C
Mol. weight [g/mol]: 293.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.28		Crippen Method
logp	3.065		Crippen Method
rinpol	1758.00		NIST Webbook
rinpol	1759.00		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=R93953&Units=SI

Legend

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