Adenosine, 2'-deoxy-N-(trimethylsilyl)-3'-O-(trimethylsilyl)-, 5'-[bis(trimethylsilyl) phosphate]

Other names:	Deoxyadenosine-5'-monophosphate (4TMS); deoxyadenosine-5'-monophosphate, TMS
Inchi:	InChI=1S/C22H46N5O6PSi4/c1-35(2,3)26-21-20-22(24-15-23-21)27(16-25-20)19-13-17(
InchiKey:	LDQVYNZLWNEILO-UHFFFAOYSA-N
Formula:	C22H46N5O6PSi4
SMILES:	C[Si](C)(C)Nc1ncnc2c1ncn2C1CC(O[Si](C)(C)C)C(COP(=O)(O[Si](C)(C)C)O[Si](C)(C)C)
Mol. weight [g/mol]:	619.95
CAS:	32645-70-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	6.408		Crippen Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32645708&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

Latest version available from:
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