

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

Other names:

5'-Adenylic acid, N-(trimethylsilyl)-2',3'-bis-O-(trimethylsilyl)-, bis(trimethylsilyl) phosphate
Adenosine-5'-monophosphate, pentakis-TMS

adenosine-5'-monophosphate, TMS

Inchi: InChI=1S/C25H54N5O7PSi5/c1-39(2,3)29-23-20-24(27-17-26-23)30(18-28-20)25-22(35-36)21-19-20
InchiKey: SUBGEEAXSQFR TK-UHFFFAOYSA-N
Formula: C25H54N5O7PSi5
SMILES: C[Si](C)(C)Nc1ncnc2c1ncn2C1OC(COP(=O)(O[Si](C)(C)C)O[Si](C)(C)C)C(O[Si](C)(C)C)C
Mol. weight [g/mol]: 708.13
CAS: 32653-14-8

Physical Properties

Property code	Value	Unit	Source
log10ws	1.31		Crippen Method
logp	7.238		Crippen Method
rinpol	3114.00		NIST Webbook
rinpol	3115.00		NIST Webbook
rinpol	3114.00		NIST Webbook
rinpol	3115.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C32653148&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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