

2'-Deoxyadenosine, N-trimethylsilyl-, bis(trimethylsilyl) ether

Other names: Adenine, deoxyriboside, TMS
Inchi: InChI=1S/C19H37N5O3Si3/c1-28(2,3)23-18-17-19(21-12-20-18)24(13-22-17)16-10-14(2
InchiKey: PSEZCYIEJIOFHY-UHFFFAOYSA-N
Formula: C19H37N5O3Si3
SMILES: C[Si](C)(C)Nc1ncnc2c1ncn2C1CC(O[Si](C)(C)C)C(CO[Si](C)(C)C)O1
Mol. weight [g/mol]: 467.79

Physical Properties

Property code	Value	Unit	Source
log10ws	0.56		Crippen Method
logp	4.432		Crippen Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
rinpol	2618.00		NIST Webbook
rinpol	2619.00		NIST Webbook
rinpol	2591.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375680&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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:

<https://www.chemeo.com/cid/18-733-8/2-Deoxyadenosine-N-trimethylsilyl-bis-trimethylsilyl-ether.pdf>

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