

9H-Purin-6-amine, N,9-bis(trimethylsilyl)-

Other names:

Adenine, N,9-bis(trimethylsilyl)-
N,9-Bis(trimethylsilyl)adenine
N-6,9-Bis(trimethylsilyl)adenine
Adenine, N,N'-bis(trimethylsilyl) ether
N-(Trimethylsilyl)-N-[9-(trimethylsilyl)-9H-purin-6-yl]amine
Adenine, N,N'-bis(trimethylsilyl)-
Adenine, bis-TMS
NSC 154617
adenine, TMS
Adenine, 2TMS
N,9-bis(trimethylsilyl)-9H-purin-6-amine
Adenine, 2tms derivative

Inchi:

InChI=1S/C11H21N5Si2/c1-17(2,3)15-10-9-11(13-7-12-10)16(8-14-9)18(4,5)6/h7-8H,1-6

InchiKey:

SSWSPDDXHGZYTU-UHFFFAOYSA-N

Formula:

C11H21N5Si2

SMILES:

C[Si](C)(C)Nc1ncnc2c1ncn2[Si](C)(C)C

Mol. weight [g/mol]:

279.49

CAS:

17995-04-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.19		Crippen Method
logp	2.756		Crippen Method
rinpol	1844.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1876.90		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1880.00		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=C17995049&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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