

CYSTATHIONINE TETRA-TMS

Other names:	CYSTATHIONINE,N,N,O,O-TMS Cystathionine, TMS Cystathionine, 4tms derivative
Inchi:	InChI=1S/C19H46N2O4SSi4/c1-27(2,3)20-16(18(22)24-29(7,8)9)13-14-26-15-17(21-28(4
InchiKey:	UCHYCIWAEYBTEB-UHFFFAOYSA-N
Formula:	C19H46N2O4SSi4
SMILES:	C[Si](C)(C)NC(CCSCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	511.00

Physical Properties

Property code	Value	Unit	Source
logp	4.452		Crippen Method
rinpol	2207.90		NIST Webbook
rinpol	2235.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U141330&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/35-166-9/CYSTATHIONINE-TETRA-TMS.pdf>

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