

L-Citrulline, N,N'-bis(trimethylsilyl)-, trimethylsilyl ester

Other names:	L-citrulline, 3tms derivative
Inchi:	InChI=1S/C15H37N3O3Si3/c1-22(2,3)17-13(14(19)21-24(7,8)9)11-10-12-16-15(20)18-23
InchiKey:	XPPZURUXPNOCEH-UHFFFAOYSA-N
Formula:	C15H37N3O3Si3
SMILES:	C[Si](C)(C)NC(=O)NCCCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	391.73

Physical Properties

Property code	Value	Unit	Source
log10ws	2.45		Crippen Method
logp	3.072		Crippen Method
rinpol	2096.50		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=U333745&Units=SI

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/54-291-9/L-Citrulline-N-N-bis-trimethylsilyl-trimethylsilyl-ester.pdf>

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