«alpha»-Aminoadipic acid, triTMS

Other names:	Hexanedioic acid, «alpha»-amino-, tri(trimethylsilyl)-
	N,O,O'-Tris-(trimethylsilyl)-2-aminoadipic acid
	2-Aminoadipic acid, N-(trimethylsilyl)-, bis(trimethylsilyl) ester
	2-Aminoadipic acid, (3TMS)
	Hexanedioic acid, «alpha»-amino, N,O,O-tris-TMS
	2-Aminoadipic acid, TMS
	HEXANEDIOIC acid, «alpha»-AMINO, N,O,O-TMS
	DL-2-Aminoadipic acid, N-(trimethylsilyl)-, bis(trimethylsilyl) ester
	2-Aminoadipic acid, 3tms derivative
Inchi:	InChI=1S/C15H35NO4Si3/c1-21(2,3)16-13(15(18)20-23(7,8)9)11-10-12-14(17)19-22(4,5
InchiKey:	RKECYUANKVVNBK-UHFFFAOYSA-N
Formula:	C15H35NO4Si3
SMILES:	C[Si](C)(C)NC(CCCC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	377.70
CAS:	66434-50-2

Physical Properties

Property code	Value	Unit	Source
log10ws	2.72		Crippen Method
logp	3.706		Crippen Method
rinpol	1694.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1694.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66434502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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