

N,O,O'-tris-(trimethylsilyl)aspartic acid

Other names:	Aspartic acid, N-(trimethylsilyl)-, bis(trimethylsilyl) ester, DL-Aspartate, tri-TMS Aspartic acid, N,O,O'-TMS Asp, tris-TMS Asp, TMS ASPARTIC ACID,N,N,O-TMS Aspartic acid, 3tms derivative
Inchi:	InChI=1S/C13H31NO4Si3/c1-19(2,3)14-11(13(16)18-21(7,8)9)10-12(15)17-20(4,5)6/h11
InchiKey:	CTMXPIJTHHSEEF-UHFFFAOYSA-N
Formula:	C13H31NO4Si3
SMILES:	C[Si](C)(C)NC(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	349.65
CAS:	15985-05-4

Physical Properties

Property code	Value	Unit	Source
log10ws	3.56		Crippen Method
logp	2.926		Crippen Method
rinpola	1530.00		NIST Webbook
rinpola	1541.00		NIST Webbook
rinpola	1530.00		NIST Webbook
ripola	1683.85		NIST Webbook
ripola	1683.85		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15985054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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