ACETYLASPARTIC ACID triTMS

Inchi:	InChI=1S/C15H33NO5Si3/c1-12(19-22(2,3)4)16-13(15(18)21-24(8,9)10)11-14(17)20-23(
InchiKey:	QVMTWZJALBUZMG-UHFFFAOYSA-N
Formula:	C15H33NO5Si3
SMILES:	CC(=NC(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]:	391.68

Physical Properties

Property code	Value	Unit	Source
log10ws	3.16		Crippen Method
logp	3.771		Crippen Method
rinpol	1680.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R395943&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/19-820-0/ACETYLASPARTIC-ACID-triTMS.pdf

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