

# ACETYLASPARTIC ACID diTMS

<b>Other names:</b>	N-Acetylaspartic acid, diTMS N-Acetylaspartic acid, bis-TMS
<b>Inchi:</b>	InChI=1S/C12H25NO5Si2/c1-9(14)13-10(12(16)18-20(5,6)7)8-11(15)17-19(2,3)4/h10H,8
<b>InchiKey:</b>	ATJCPJZSHSEVIW-UHFFFAOYSA-N
<b>Formula:</b>	C12H25NO5Si2
<b>SMILES:</b>	CC(=O)NC(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	319.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	2.25		Crippen Method
logp	1.637		Crippen Method
rinpol	1640.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1640.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R273393&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R273393&amp;Units=SI</a>

## Legend

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

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