

# N-Methyl-3,4-dihydroxyphenylalanine, N-TFA-O-TMS

<b>Inchi:</b>	InChI=1S/C21H36F3NO5Si3/c1-25(20(27)21(22,23)24)16(19(26)30-33(8,9)10)13-15-11-
<b>InchiKey:</b>	YHZNNDRWAXPVG-P-UHFFFAOYSA-N
<b>Formula:</b>	C21H36F3NO5Si3
<b>SMILES:</b>	CN(C(=O)C(F)(F)F)C(Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)C(=O)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	523.77

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	5.424		Crippen Method
rinpol	2165.00		NIST Webbook

## Sources

<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=R139189&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R139189&amp;Units=SI</a>
<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>

## 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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