

# 2-[[tert-Butyl(dimethyl)silyl](methyl)amino]-1-(4-pyrr

<b>Other names:</b>	2-[[tert-Butyl(dimethyl)silyl](methyl)amino]-1-(4-[[tert-butyl(dimethyl)silyl]oxy]-3-methoxy)pyrrolidine Metanephrine, n-2tdms derivative
<b>Inchi:</b>	InChI=1S/C22H43NO3Si2/c1-21(2,3)27(9,10)23(7)16-18(24)17-13-14-19(20(15-17)25-8)
<b>InchiKey:</b>	IDSR SXAUPMIXDC-UHFFFAOYSA-N
<b>Formula:</b>	C22H43NO3Si2
<b>SMILES:</b>	COc1cc(C(O)CN(C)[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	425.75

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	6.050		Crippen Method
rinpol	2534.20		NIST Webbook
rinpol	2534.20		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=U334025&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U334025&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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