

# N-(Trifluoroacetyl)-O,O',O''-tris(trimethylsilyl)epinephrine

<b>Other names:</b>	Adrenaline, N-TFA-tris-(O-TMS) Adrenaline, N-TFA-O-TMS
<b>Inchi:</b>	InChI=1S/C20H36F3NO4Si3/c1-24(19(25)20(21,22)23)14-18(28-31(8,9)10)15-11-12-16(
<b>InchiKey:</b>	SXAPUNOGPVDUQY-UHFFFAOYSA-N
<b>Formula:</b>	C20H36F3NO4Si3
<b>SMILES:</b>	CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1)C(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	495.76
<b>CAS:</b>	54135-51-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.59		Crippen Method
logp	6.027		Crippen Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		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=C54135512&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54135512&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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