

# Butane, 1,2,4-tris(trimethylsiloxy)-

<b>Other names:</b>	butane-1,2,4-triol, TMS
<b>Inchi:</b>	InChI=1S/C13H34O3Si3/c1-17(2,3)14-11-10-13(16-19(7,8)9)12-15-18(4,5)6/h13H,10-12H
<b>InchiKey:</b>	ZWTQGTCQGKKVSN-UHFFFAOYSA-N
<b>Formula:</b>	C13H34O3Si3
<b>SMILES:</b>	C[Si](C)(C)OCCC(CO[Si](C)(C)C)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	322.66
<b>CAS:</b>	33581-75-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.21		Crippen Method
logp	4.300		Crippen Method
rinpol	1353.60		NIST Webbook
rinpol	1353.60		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C33581758&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33581758&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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<https://www.chemeo.com/cid/119-889-4/Butane-1-2-4-tris-trimethylsiloxy.pdf>

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