

# Benzenepropanoic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester

<b>Other names:</b>	Trimethylsilyl m-trimethylsiloxyphenylpropionate 3-(3-Hydroxyphenyl)propionic acid, di(trimethylsilyl)- 3-Hydroxyphenylpropionic acid, di-TMS Benzenepropanoic acid, 3-hydroxy, bis-TMS Benzenepropanoic acid, 3-hydroxy, TMS 3-(3-Hydroxyphenyl)propanoic acid, 2tms derivative
<b>Inchi:</b>	InChI=1S/C15H26O3Si2/c1-19(2,3)17-14-9-7-8-13(12-14)10-11-15(16)18-20(4,5)6/h7-9,
<b>InchiKey:</b>	IEMLASUXNKHKEZ-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O3Si2
<b>SMILES:</b>	C[Si](C)(C)OC(=O)CCc1ccc(O[Si](C)(C)C)c1
<b>Mol. weight [g/mol]:</b>	310.54
<b>CAS:</b>	55887-87-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.13		Crippen Method
logp	4.211		Crippen Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1738.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55887871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55887871&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

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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