

# o-Vanilline, MO TMS

Inchi:	InChI=1S/C12H19NO3Si/c1-14-12-10(9-13-15-2)7-6-8-11(12)16-17(3,4)5/h6-9H,1-5H3/b
InchiKey:	JOYXHEXUVYKKCY-LCYFTJDESA-N
Formula:	C12H19NO3Si
SMILES:	CON=Cc1cccc(O[Si](C)(C)C)c1OC
Mol. weight [g/mol]:	253.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.75		Crippen Method
logp	2.889		Crippen Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R92616&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R92616&amp;Units=SI</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/24-134-6/o-Vanilline-MO-TMS.pdf>

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