

3-VANILPROPANOL, BIS(TRIMETHYLSILYL)-DERIV.

Other names:	1-Propanol, 3-(4-hydroxy-3-methoxyphenyl), bis-TMS
Inchi:	InChI=1S/C16H30O3Si2/c1-17-16-13-14(9-8-12-18-20(2,3)4)10-11-15(16)19-21(5,6)7/h1
InchiKey:	TVSUPPZPVDKCMU-UHFFFAOYSA-N
Formula:	C16H30O3Si2
SMILES:	COc1cc(CCCO[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	326.58

Physical Properties

Property code	Value	Unit	Source
ie	8.28	eV	Cheméo Relay (1.0)
logp	4.693		Crippen Method
rinpol	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U79076&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/82-294-5/3-VANILPROPANOL-BIS-TRIMETHYLSILYL-DERIV.pdf>

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