

Vanillin, tert-butyldimethylsilyl ether

Other names:	Vanillin, tbdms derivative
Inchi:	InChI=1S/C14H22O3Si/c1-14(2,3)18(5,6)17-12-8-7-11(10-15)9-13(12)16-4/h7-10H,1-6H3
InchiKey:	UBTYFBWZR XUZZFF-UHFFFAOYSA-N
Formula:	C14H22O3Si
SMILES:	COc1cc(C=O)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	266.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	3.892		Crippen Method
rinpol	1796.10		NIST Webbook
rinpol	1796.10		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352846&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/115-624-1/Vanillin-tert-butyldimethylsilyl-ether.pdf>

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