

4'-Hydroxy-3'-methoxyacetophenone, tert-butyl dimethylsilyl ether

Other names:	Acetovanillone, tbdms derivative
Inchi:	InChI=1S/C15H24O3Si/c1-11(16)12-8-9-13(14(10-12)17-5)18-19(6,7)15(2,3)4/h8-10H,1-
InchiKey:	APNKCPNBQQKLDJ-UHFFFAOYSA-N
Formula:	C15H24O3Si
SMILES:	COc1cc(C(C)=O)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	280.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	4.282		Crippen Method
rinpol	1877.60		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/91-186-5/4-Hydroxy-3-methoxyacetophenone-tert-butyl dimethylsilyl-ether.pdf>

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