

# Warfarin, tert-butyldimethylsilyl ether

<b>Other names:</b>	Warfarin, tbdms derivative
<b>Inchi:</b>	InChI=1S/C25H30O4Si/c1-17(26)16-20(18-12-8-7-9-13-18)22-23(29-30(5,6)25(2,3)4)19-
<b>InchiKey:</b>	LVUJUTVWDLBSD-UHFFFAOYSA-N
<b>Formula:</b>	C25H30O4Si
<b>SMILES:</b>	CC(=O)CC(c1ccccc1)c1c(O[Si](C)(C)C(C)(C)C)c2ccccc2oc1=O
<b>Mol. weight [g/mol]:</b>	422.59

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.30		Crippen Method
logp	6.288		Crippen Method
rinpol	2935.50		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333974&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333974&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>

## Legend

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

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<https://www.chemeo.com/cid/12-403-0/Warfarin-tert-butyldimethylsilyl-ether.pdf>

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