

# Benzoic acid, 2-hydroxy-3-methoxycarbonyl, DTBS

<b>Inchi:</b>	InChI=1S/C17H24O5Si/c1-16(2,3)23(17(4,5)6)21-13-11(14(18)20-7)9-8-10-12(13)15(19)
<b>InchiKey:</b>	QNRVGUQFEJCZGN-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O5Si
<b>SMILES:</b>	<chem>COC(=O)c1cccc2c1O[Si](C(C)(C)C)(C(C)(C)C)OC2=O</chem>
<b>Mol. weight [g/mol]:</b>	336.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	4.065		Crippen Method
rinpol	2000.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R41182&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R41182&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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