

# Benzylmalic acid, TBDMS

<b>Inchi:</b>	InChI=1S/C29H54O5Si3/c1-27(2,3)35(10,11)32-24(26(31)34-37(14,15)29(7,8)9)23(21-22
<b>InchiKey:</b>	SERKHULUKJGTSC-UHFFFAOYSA-N
<b>Formula:</b>	C29H54O5Si3
<b>SMILES:</b>	CC(C)(C)[Si](C)(C)OC(=O)C(Cc1ccccc1)C(O[Si](C)(C)C(C)(C)C(=O)O[Si](C)(C)C(C)(C
<b>Mol. weight [g/mol]:</b>	566.99

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	8.332		Crippen Method
rinpol	2217.00		NIST Webbook
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## 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=R564000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R564000&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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/36-910-1/Benzylmalic-acid-TBDMS.pdf>

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