

# 1-O-trans-p-Coumaroylglycerol, 3TMS

<b>Inchi:</b>	InChI=1S/C21H38O5Si3/c1-27(2,3)24-17-20(26-29(7,8)9)16-23-21(22)15-12-18-10-13-1
<b>InchiKey:</b>	XIKYLENERWEDIW-NTCAYCPXSA-N
<b>Formula:</b>	C21H38O5Si3
<b>SMILES:</b>	C[Si](C)(C)OCC(COC(=O)C=Cc1ccc(O[Si](C)(C)C)cc1)O[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	454.78
<b>CAS:</b>	1048040-87-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	1.26		Crippen Method
logp	5.528		Crippen Method
rinpola	2494.60		NIST Webbook
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## Sources

<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.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=C1048040874&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1048040874&amp;Units=SI</a>

## Legend

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

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