

Sinapic alcohol, TMS

Other names:	SINAPINYL ALCOHOL (2TMS) SINAPYL ALCOHOL 2TMS
Inchi:	InChI=1S/C17H30O4Si2/c1-18-15-12-14(10-9-11-20-22(3,4)5)13-16(19-2)17(15)21-23(6
InchiKey:	GYQFNHIVJPYRJM-MDZDMXLPSA-N
Formula:	C17H30O4Si2
SMILES:	COc1cc(C=CCO[Si](C)(C)C)cc(OC)c1O[Si](C)(C)C
Mol. weight [g/mol]:	354.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.36		Crippen Method
logp	4.782		Crippen Method
rinpola	2051.60		NIST Webbook
rinpola	2051.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R247582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/19-180-1/Sinapic-alcohol-TMS.pdf>

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