Flavanone, 5,4'-dihydroxy-7-methoxy, bis-TMS

Other names:	Sakuranetin, TMS
Inchi:	InChI=1S/C22H30O5Si2/c1-24-17-12-20-22(21(13-17)27-29(5,6)7)18(23)14-19(25-20)15
InchiKey:	JQRKEUQHRRUNLY-UHFFFAOYSA-N
Formula:	C22H30O5Si2
SMILES:	COc1cc2c(c(O[Si](C)(C)C)c1)C(=O)CC(c1ccc(O[Si](C)(C)C)cc1)O2
Mol. weight [g/mol]:	430.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	5.829		Crippen Method
rinpol	2818.00		NIST Webbook
rinpol	2818.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R936&Units=SI

Legend

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

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