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