Chrysin, bis(trimethylsilyl) ether

Other names:	Flavone, 5,7-dihydroxy, TMS
	Flavone, 5,7-dihydroxy, bis-TMS
	5,7-Dihydroxyflavone, bis-TMS
	Chrysin, 2tms derivative
Inchi:	InChI=1S/C21H26O4Si2/c1-26(2,3)24-16-12-19-21(20(13-16)25-27(4,5)6)17(22)14-18(23
InchiKey:	GIBLMWDGNJTUAZ-UHFFFAOYSA-N
Formula:	C21H26O4Si2
SMILES:	C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c2c(=O)cc(-c3ccccc3)oc2c1
Mol. weight [g/mol]:	398.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.05		Crippen Method
logp	5.887		Crippen Method
rinpol	2705.00		NIST Webbook
rinpol	2704.00		NIST Webbook
rinpol	2704.00		NIST Webbook
rinpol	2694.00		NIST Webbook
rinpol	2694.00		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=U333499&Units=SI

Legend

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