Quercetin, 5,7,3',4'-tetra-TMS

Inchi: InChI=1S/C27H42O7Si4/c1-35(2,3)31-19-16-22-24(23(17-19)34-38(10,11)12)25(28)26(2
InchiKey: XSFIYZIIRKXSBC-UHFFFAOYSA-N
Formula: C27H42O7Si4
SMILES: C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c2c(=O)c(O)c(-c3ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c3)oc2
Mol. weight [g/mol]: 590.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	8.020		Crippen Method
rinpol	3011.00		NIST Webbook
rinpol	3011.00		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=R572457&Units=SI

Legend

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