Quercetin (5TMS)

Inchi: InChI=1S/C30H50O7Si5/c1-38(2,3)33-22-19-25-27(26(20-22)36-41(10,11)12)28(31)30(3
InchiKey: VISLTJDFZRIFEA-UHFFFAOYSA-N
Formula: C30H50O7Si5
SMILES: C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c2c(=O)c(O[Si](C)(C)C)c(-c3ccc(O[Si](C)(C)C)c(O[Si](C)(
Mol. weight [g/mol]: 663.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	9.528		Crippen Method
rinpol	3164.00		NIST Webbook
rinpol	3164.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U413966&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
rinpol: Non-polar retention indices