Apigenin, TMS

Other names: APIGENIN 3TMS
Flavone, 4',5,7-trihydroxy, TMS
Inchi: InChI=1S/C24H34O5Si3/c1-30(2,3)27-18-12-10-17(11-13-18)21-16-20(25)24-22(26-21)1
InchiKey: CCZQELBLBRCVLH-UHFFFAOYSA-N
Formula: C24H34O5Si3
SMILES: C[Si](C)(C)Oc1ccc(-c2cc(=O)c3c(O[Si](C)(C)C)cc(O[Si](C)(C)C)cc3o2)cc1
Mol. weight [g/mol]: 486.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	7.101		Crippen Method
rinpol	3142.20		NIST Webbook
rinpol	3137.50		NIST Webbook
rinpol	3128.00		NIST Webbook
rinpol	3128.00		NIST Webbook
rinpol	3137.50		NIST Webbook
rinpol	3142.20		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R7757&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