4',5,7-Trihydroxyflavanone, tris(trimethylsilyl) ether

Other names: Naringenin, TMS
Flavanone, 5,7,4'-trihydroxy, tris-TMS
NARINGENIN 3TMS-1
Naringenin, 3tms derivative

Inchi: InChI=1S/C24H36O5Si3/c1-30(2,3)27-18-12-10-17(11-13-18)21-16-20(25)24-22(26-21)1

InchiKey: ZMEWYEXWOABPGS-UHFFFAOYSA-N

Formula: C24H36O5Si3

SMILES: C[Si](C)(C)Oc1ccc(C2CC(=O)c3c(cc(O[Si](C)(C)C)cc3O[Si](C)(C)C)O2)cc1

Mol. weight [g/mol]: 488.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.24		Crippen Method
logp	7.034		Crippen Method
rinpol	2861.80		NIST Webbook
rinpol	2907.90		NIST Webbook
rinpol	2851.00		NIST Webbook
rinpol	2843.00		NIST Webbook
rinpol	2843.00		NIST Webbook
rinpol	2872.20		NIST Webbook
rinpol	2851.00		NIST Webbook
rinpol	2861.80		NIST Webbook
rinpol	2872.20		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333498&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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