Flavanone, 5,7-dihydroxy, TMS

Other names: Pinocembrin, TMS
Flavanone, 5,7-dihydroxy, bis-TMS
Inchi: InChI=1S/C21H28O4Si2/c1-26(2,3)24-16-12-19-21(20(13-16)25-27(4,5)6)17(22)14-18(23
InchiKey: GEFWTBJOQNFPFG-UHFFFAOYSA-N
Formula: C21H28O4Si2
SMILES: C[Si](C)(C)Oc1cc2c(c(O[Si](C)(C)C)c1)C(=O)CC(c1ccccc1)O2
Mol. weight [g/mol]: 400.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	5.821		Crippen Method
rinpol	2507.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook
rinpol	2492.00		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=R46374&Units=SI

Legend

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