GA81, Me-TMS

Other names: GA81, MeTMSi
Inchi: InChI=1S/C26H42O6Si2/c1-16-12-24-15-25(16,32-34(7,8)9)11-10-18(24)26-14-17(31-33
InchiKey: AINOJINHOWCGRJ-LCQZQDNUSA-N
Formula: C26H42O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CC(O[Si](C)(C)C)CC(C)(C(=O)O1)C2C3C(=O)C
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	5.058		Crippen Method
rinpol	2666.00		NIST Webbook
rinpol	2673.00		NIST Webbook
rinpol	2682.00		NIST Webbook
rinpol	2698.00		NIST Webbook
rinpol	2683.00		NIST Webbook
rinpol	2687.00		NIST Webbook
rinpol	2694.00		NIST Webbook
rinpol	2681.00		NIST Webbook
rinpol	2694.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R79985&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