GA87, MeTMSi

Other names: GA87, MeTMS
Inchi: InChI=1S/C29H48O7Si3/c1-18-16-27-17-29(18,36-39(10,11)12)21(35-38(7,8)9)15-19(27
InchiKey: CODGHIRYLJNHPK-MFBNQEKNSA-N
Formula: C29H48O7Si3
SMILES: C=C1CC23CC1(O[Si](C)(C)C)C(O[Si](C)(C)C)CC2C12C=CC(O[Si](C)(C)C)C(C)(C(=O)C
Mol. weight [g/mol]: 592.94

Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	5.664		Crippen Method
rinpol	2848.00		NIST Webbook
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
rinpol	2854.00		NIST Webbook
rinpol	2853.00		NIST Webbook
rinpol	2894.00		NIST Webbook
rinpol	2895.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R80045&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