GA18, MeTMS

Inchi:	InChI=1S/C28H48O6Si2/c1-18-16-27-17-28(18,34-36(9,10)11)15-12-19(27)25(2)14-13-2
InchiKey:	MDTYDUOSWPVURF-GREOGJAMSA-N
Formula:	C28H48O6Si2
SMILES:	C=C1CC23CC1(O[Si](C)(C)C)CCC2C1(C)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=C
Mol. weight [g/mol]:	536.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	5.942		Crippen Method
rinpol	2646.00		NIST Webbook
rinpol	2654.00		NIST Webbook
rinpol	2656.00		NIST Webbook
rinpol	2624.00		NIST Webbook
rinpol	2646.00		NIST Webbook
rinpol	2654.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R79266&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

Latest version available from:
https://www.chemeo.com/cid/35-691-6/GA18-MeTMS.pdf

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