cis-Isoadhumulone, TMS

Inchi:	InChI=1S/C27H46O5Si2/c1-13-20(6)24(29)23-25(30)21(16-14-18(2)3)27(32-34(10,11)12
InchiKey:	QHGGPAUBGUQBCS-COWGUHPFSA-N
Formula:	C27H46O5Si2
SMILES:	CCC(C)C(=O)C1=C(O[Si](C)(C)C)C(O[Si](C)(C)C)(C(=O)CC=C(C)C)C(CC=C(C)C)C1=C
Mol. weight [g/mol]:	506.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	6.778		Crippen Method
rinpol	2652.00		NIST Webbook
rinpol	2603.00		NIST Webbook
rinpol	2652.00		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=R96959&Units=SI

Legend

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

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