trans-Isohumulone, TMS

Inchi:	InChI=1S/C29H54O4Si3/c1-21(2)16-17-24-27(30)26(25(20-23(5)6)31-34(7,8)9)28(32-35
InchiKey:	XFHXXWFFWSCATK-WVYFDLHMSA-N
Formula:	C29H54O4Si3
SMILES:	CC(C)=CCC1C(=O)C(C(=CC(C)C)O[Si](C)(C)C)=C(O[Si](C)(C)C)C1(CC=C(C)C)O[Si](C
Mol. weight [g/mol]:	550.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	8.985		Crippen Method
rinpol	2629.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2629.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R97143&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

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