Brassicasterol, TMS

Inchi:	InChI=1S/C31H54OSi/c1-21(2)22(3)10-11-23(4)27-14-15-28-26-13-12-24-20-25(32-33(7
InchiKey:	OUZPLOOSCBQQGW-ITLMFHBGSA-N
Formula:	C31H54OSi
SMILES:	CC(C)C(C)C=CC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	470.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	9.270		Crippen Method
rinpol	3185.00		NIST Webbook
rinpol	3185.00		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=R528940&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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