

19-Nor-5,7,9(10)-cholestatrien-3«beta»-ol, TMS

Inchi:	InChI=1S/C29H48OSi/c1-20(2)9-8-10-21(3)27-15-16-28-26-13-11-22-19-23(30-31(5,6)7)
InchiKey:	HAYHXZDJTAFLEW-QGJQKYCNSA-N
Formula:	C29H48OSi
SMILES:	CC(C)CCCC(C)C1CCC2c3ccc4c(c3CCC21C)CCC(O[Si](C)(C)C)C4
Mol. weight [g/mol]:	440.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.89		Crippen Method
logp	8.304		Crippen Method
rinpol	3206.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R390948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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<https://www.chemeo.com/cid/59-525-4/19-Nor-5-7-9-10-cholestatrien-3-beta-ol-TMS.pdf>

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