

5,6«alpha»-epoxysitosterol, TMS

Inchi: InChI=1S/C32H58O2Si/c1-10-23(21(2)3)12-11-22(4)26-13-14-27-25-19-29-32(33-29)20-
InchiKey: XMBJXERAHCFWDD-CJOAZAGBSA-N
Formula: C32H58O2Si
SMILES: CCC(CCC(C)C1CCC2C3CC4OC45CC(O[Si](C)(C)C)CCC5(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 502.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.08		Crippen Method
logp	9.095		Crippen Method
rinpol	3431.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395374&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/45-432-2/5-6-alpha-epoxysitosterol-TMS.pdf>

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