

Episterol 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: BVQJSEUNJXEAJ-SBBLNQPISA-N
Formula: C₃₁H₅₄OSi
SMILES: C=C(CCC(C)C1CCC2C3=CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]: 470.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.40		Crippen Method
logp	9.414		Crippen Method
rinpol	3272.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R273006&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/41-623-4/Episterol-TMS.pdf>

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