

Epicholesterol, TBDMSi (3-O)

Inchi: InChI=1S/C33H60OSi/c1-23(2)12-11-13-24(3)28-16-17-29-27-15-14-25-22-26(34-35(9,10)36-37)31-32
InchiKey: CXIGRSVIJKSIQL-MPYHSKAUSA-N
Formula: C33H60OSi
SMILES: CC(C)CCCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 500.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.39		Crippen Method
logp	10.418		Crippen Method
rinpol	3273.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R144651&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.cheméo.com/cid/34-177-8/Epicholesterol-TBDMSi-3-O.pdf>

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