5«beta»-Cholane-3«alpha»,7«alpha»,24-triol, TMS

Inchi: InChI=1S/C33H66O3Si3/c1-24(14-13-21-34-37(4,5)6)27-15-16-28-31-29(18-20-33(27,28

InchiKey: DIDRNKWXXWKOIP-PRCCELAASA-N

Formula: C33H66O3Si3

SMILES: CC(CCCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC

Mol. weight [g/mol]: 595.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	9.963		Crippen Method
rinpol	3298.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R271644&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/52-766-4/5-beta-Cholane-3-alpha-7-alpha-24-triol-TMS.pdf

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