Deoxycholic acid, tris(trimethylsilyl) deriv.

Other names: 3«alpha»,12«alpha»-dihydroxy-5«beta»-cholan-24-oic acid, TMS
Inchi: InChI=1S/C33H64O4Si3/c1-23(13-18-31(34)37-40(10,11)12)27-16-17-28-26-15-14-24-21
InchiKey: GUYGBOQSRRUZIK-UHFFFAOYSA-N
Formula: C33H64O4Si3
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C
Mol. weight [g/mol]: 609.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	9.490		Crippen Method
rinpol	3207.00		NIST Webbook
rinpol	3212.00		NIST Webbook
rinpol	3207.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U365565&Units=SI

Legend

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