

3«beta»,7«beta»-Dihydroxy-5«beta»-cholanoic acid, MeTMS

Other names:

thoursodeoxycholic acid, trimethylsilyl ether-methyl ester

Inchi: InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3

InchiKey: FUVKOFYYHKWFJK-MLZFRZJBSA-N

Formula: C31H58O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12O

Mol. weight [g/mol]: 550.96

CAS: 78964-21-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3316.00		NIST Webbook
rinpol	3268.00		NIST Webbook
rinpol	3316.00		NIST Webbook
rinpol	3268.00		NIST Webbook
ripol	3687.00		NIST Webbook
ripol	3687.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C78964213&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
ripol: Polar retention indices

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