

3-«alpha»,7-«alpha»,12-«alpha»-Trihydroxy-nor-5- acid, MeTMS

Inchi: COC(=O)CC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1
InchiKey: IQRHCEGIECHWFO-SIBKOBOISA-N
Formula: C33H64O5Si3
SMILES: COC(=O)CC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 625.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	8.725		Crippen Method

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=R393190&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

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