Androstenetriol MO TMS

Inchi: InChI=1S/C28H54O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)19-24(30-33(6,7)8)26-22-
InchiKey: YZJWSRYSQHTCFY-ZGEFQZNXSA-N
Formula: C28H54O3Si3
SMILES: CC12CCC(O[Si](C)(C)C)CC1=CC(O[Si](C)(C)C)C1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 522.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	8.219		Crippen Method
rinpol	2865.00		NIST Webbook
rinpol	2868.00		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
rinpol	2868.00		NIST Webbook
rinpol	2859.00		NIST Webbook
rinpol	2840.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R97634&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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