Pregnanetriol MO TMS

Inchi: InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)24-13-14-25-28-26(16-18-30(24,25)3)29(2)1
InchiKey: ANLFUEQWODEQDA-BOUGQGRLSA-N
Formula: C30H60O3Si3
SMILES: CC(O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
logp	8.935		Crippen Method
rinpol	2832.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2819.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2828.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R97670&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/43-715-0/Pregnanetriol-MO-TMS.pdf

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