

5,6«alpha»-22,23-diepoxytigmasterol, TMS, II

Inchi: InChI=1S/C32H56O3Si/c1-10-22(19(2)3)29-28(33-29)20(4)24-11-12-25-23-17-27-32(34-35)21-6-7-8-9-5-2
InchiKey: KHCUMNVQUIJUOP-ZGIOHZBTSA-N
Formula: C32H56O3Si
SMILES: CCC(C(C)C)C1OC1C(C)C1CCC2C3CC4OC45CC(O[Si](C)(C)C)CCC5(C)C3CCC12C
Mol. weight [g/mol]: 516.87

Physical Properties

Property code	Value	Unit	Source
logp	8.082		Crippen Method
rinpol	3551.00		NIST Webbook
rinpol	3551.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395354&Units=SI>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/94-701-9/5-6-alpha-22-23-diepoxytigmasterol-TMS-II.pdf>

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