

iso-12«alpha»-hydroxy-GA43 methyl ester TMS ether

Inchi: InChI=1S/C32H56O9Si3/c1-19-16-31-17-20(19)21(39-42(6,7)8)15-23(31)32(29(35)38-5)
InchiKey: PVBQNJGVDDQATAE-FNWJYIFCSA-N
Formula: C32H56O9Si3
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C(=O)OC)CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C)
Mol. weight [g/mol]: 669.04

Physical Properties

Property code	Value	Unit	Source
logp	5.781		Crippen Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177087&Units=SI>
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):

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/116-199-3/iso-12-alpha-hydroxy-GA43-methyl-ester-TMS-ether.pdf>

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