

12«beta»-OH-GA51 methyl ester TMS ether

Inchi: InChI=1S/C26H42O6Si2/c1-15-11-25-14-17(15)18(32-34(7,8)9)10-19(25)26-13-16(31-33)
InchiKey: NMRYFGCLCMKNFO-GOOSAKOESA-N
Formula: C₂₆H₄₂O₆Si₂
SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CC(O[Si](C)(C)C)CC(C)(C(=O)O1)C2C3C(=O)C
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	4.914		Crippen Method
rinpol	2649.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R151763&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/32-408-3/12-beta-OH-GA51-methyl-ester-TMS-ether.pdf>

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