

18-OH-GA47 methyl ester TMS ether

Inchi: InChI=1S/C28H48O7Si3/c1-17-14-26-15-18(17)12-13-20(26)27-16-19(33-36(3,4)5)23(34)
InchiKey: CUVRUBQOMOAVCV-IDCUGVNISA-N
Formula: C₂₈H₄₈O₇Si₃
SMILES: C=C1CC23CC1CCC2C12CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)(C(=O)O1)C
Mol. weight [g/mol]: 580.93

Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	5.498		Crippen Method
rinpol	2710.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R151807&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/47-243-0/18-OH-GA47-methyl-ester-TMS-ether.pdf>

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