

18-OH-GA48, methyl ester TMS ether

Inchi: InChI=1S/C31H56O8Si4/c1-19-16-29-17-20(19)15-21(36-40(3,4)5)24(29)30-18-22(37-41)
InchiKey: URIBOLRFEKBSKN-ODKODSMZSA-N
Formula: C31H56O8Si4
SMILES: C=C1CC23CC1CC(O[Si](C)(C)C)C2C12CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)
Mol. weight [g/mol]: 669.11

Physical Properties

Property code	Value	Unit	Source
log10ws	2.24		Crippen Method
logp	6.328		Crippen Method
rinpol	2900.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R151812&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/48-611-0/18-OH-GA48-methyl-ester-TMS-ether.pdf>

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