

19-Hydroxy PGA2 TMS

Inchi: InChI=1S/C29H54O5Si3/c1-24(32-35(2,3)4)16-15-17-26(33-36(5,6)7)22-20-25-21-23-28
InchiKey: KQXKPQPGCZDELS-NYGYWKERSA-N
Formula: C29H54O5Si3
SMILES: CC(CCCC(C=CC1C=CC(=O)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 566.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.63		Crippen Method
logp	8.039		Crippen Method
rinpol	3229.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R16787&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/40-862-0/19-Hydroxy-PGA2-TMS.pdf>

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