

PGF 1B, TMS

Inchi: InChI=1S/C32H68O5Si4/c1-14-15-18-21-27(34-38(2,3)4)24-25-29-28(22-19-16-17-20-23
InchiKey: FKCQXUAYSIAIKMH-UYCPXGDLSA-N
Formula: C32H68O5Si4
SMILES: CCCCCC(C=CC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CCCCCCC(=O)O[Si](C)(C)C)O[Si]
Mol. weight [g/mol]: 645.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.15		Crippen Method
logp	10.138		Crippen Method
rinpol	2675.00		NIST Webbook
rinpol	2699.00		NIST Webbook
rinpol	2675.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581961&Units=SI>

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/123-101-2/PGF-1B-TMS.pdf>

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