

PGF 3A, TMS

Inchi: InChI=1S/C32H64O5Si4/c1-14-15-18-21-27(34-38(2,3)4)24-25-29-28(22-19-16-17-20-23)
InchiKey: IETWKNBKTVCSD-HEACAIAQSA-N
Formula: C32H64O5Si4
SMILES: CCC=CCC(C=CC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O
Mol. weight [g/mol]: 641.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.85		Crippen Method
logp	9.690		Crippen Method
rinpol	2705.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581996&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/116-501-6/PGF-3A-TMS.pdf>

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