

PGA2 TMS

Inchi: InChI=1S/C32H66O5Si4/c1-14-15-18-21-27(34-38(2,3)4)24-25-29-28(22-19-16-17-20-23)4
InchiKey: ZWRMXRMPDPQJCB-YVPHRHBOSA-N
Formula: C32H66O5Si4
SMILES: CCCCCC(C=CC1C(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 643.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Crippen Method
logp	9.914		Crippen Method
rinpole	3038.00		NIST Webbook
rinpole	3038.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R16830&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/31-151-9/PGA2-TMS.pdf>

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