Propyl glucuronide, TMS

Inchi: InChI=1S/C21H48O7Si4/c1-14-15-23-21-19(27-31(8,9)10)17(26-30(5,6)7)16(25-29(2,3)4
InchiKey: RGPKXUCUWGYNNC-UHFFFAOYSA-N
Formula: C21H48O7Si4
SMILES: CCCOC1OC(C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 524.94

Physical Properties

Property code	Value	Unit	Source
log10ws	3.94		Crippen Method
logp	5.176		Crippen Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R554677&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