Raffinose, 11TMS

Inchi: InChI=1S/C50H118O16Si11/c1-67(2,3)52-35-38-40(59-70(10,11)12)46(65-76(28,29)30)5
InchiKey: JTNFEKSQMXJAOR-HBNHOZJJSA-N
Formula: C50H118O16Si11
SMILES: C[Si](C)(C)OCC1OC(CO[Si](C)(C)C)(OC2OC(COC3OC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(
Mol. weight [g/mol]: 1284.40

Physical Properties

Property code	Value	Unit	Source
log10ws	12.06		Crippen Method
logp	12.837		Crippen Method
rinpol	3345.00		NIST Webbook
rinpol	3396.00		NIST Webbook
rinpol	3345.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R605339&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