Laminaritriose: bD-Glcp(1->3)-bDGlcp(1->3)-DGlc, oxime-TMS, isomer # 1

Inchi: InChI=1S/C54H129NO16Si12/c1-72(2,3)56-38-42-45(61-54-52(70-82(31,32)33)50(68-80

InchiKey: HSCPKJOFDBMNBE-ZOBWJYGWSA-N

Formula: C54H129NO16Si12

SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C(OC1OC(CO[Si](C)(C)C)C(OC2OC(CO[Si](C)(C)C)C(O[S

Mol. weight [g/mol]: 1385.63

Physical Properties

Property code	Value	Unit	Source
log10ws	13.07		Crippen Method
logp	14.359		Crippen Method
rinpol	3461.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R588893&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

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https://www.chemeo.com/cid/54-195-6/Laminaritriose-bD-Glcp-1-3-bDGlcp-1-3-DGlc-oxime-TMS-isomer-1.pdf

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